

MEMORANDUM REPORT ARBRL-MR-03362

A MEFF USER'S GUIDE

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## I. INTRODUCTION

Secondary muzzle flash results from the reignition of hot, fuel-rich gun muzzle exhaust gases when they mix with air after the gun projectile is launched. Secondary muzzle flash has several deleterious effects, so that there have been continuing efforts to learn to model, predict, and suppress it. The Yousefian flash prediction model, which includes the Muzzle Exhaust Flow Field (MEFF) program<sup>1</sup>, is the only operational flash prediction model that takes detailed chemistry into account. If one wants to predict the effect of a new suppressant combination or of a new propellant composition, the Yousefian model is the only game in town.

The name MEFF is used by its author to describe both the front-end program which models the gun muzzle exhaust flow field and the overall modeling procedure, which includes the Low-Altitude Plume Prediction (LAPP) model.<sup>2</sup> LAPP contains the detailed chemical modeling; and MEFF was written to produce rational input parameters for LAPP in a fashion that changes appropriately with changes in gun parameters. MEFF is a "gun input" to LAPP, if you would. In this report, I shall attempt to confine my use of the name MEFF to descriptions of the muzzle exhaust flow field program, with the term "Yousefian model" used to describe MEFF, LAPP, and their associated programs.

The physics described by MEFF is well documented, and the reader is referred to Reference 1 for questions concerning the reasons MEFF is written the way it is. MEFF starts with the equations derived by Corner;<sup>3</sup> one resulting limitation of the code is that it is limited to cases for which the charge weight is significantly less than the projectile weight. Thus, MEFF cannot be used to model most high-velocity guns, such as those on tanks.

There are several discrete steps involved in using the Yousefian model, and not all of them are obvious. This report is intended to provide a well-described path for intelligent MEFF/LAPP utilization; one should be able to get the desired results correctly and quickly by following this guide. As an aid to understanding, a sample calculation is followed from beginning to end, and all the input and output are discussed thoroughly.

Four programs are essential to the Yousefian model. First, one needs a thermodynamics code; BLAKE<sup>4</sup> is used throughout this report, but NASA-LEWIS

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1. V. Yousefian, "Muzzle Flash Onset," ARI-RR-236, Aerodyne Research, Inc., Billerica, MA, November 1980. Also available as ARBRL-CR-00477, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, February 1982 (AD B063 573L).

2. R. R. Mikatarian, C. J. Kau, and H. S. Pergament, "A Fast Computer Program for Nonequilibrium Rocket Plume Predictions," AFRPL-TR-72-94, Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, CA, August 1972.

3. J. Corner, Theory of Interior Ballistics of Guns, John Wiley & Sons, New York (1950).

4. E. Freedman, "BLAKE - A Thermodynamic Code Based on TIGER: User's Guide and Manual," ARBRL-TR-02411, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1982 (AD A121 259).

could have been used. This report contains enough details for an experienced BLAKE user to get the desired results; a novice will probably have to get help using BLAKE. The thermodynamics code is used twice, for two separate functions. Second, an interior ballistics code is used; I have here used IBHVG, a modern version of the Baer-Frankle lumped-parameter model.<sup>5</sup> This report contains enough details for an occasional IBHVG user to get the desired results; a novice will have to get help running IBHVG. MEFF is needed as the third major step, and the information in this report is intended to be sufficient to run MEFF. Finally, LAPP<sup>2</sup> is needed; and again, the information in this report should be all a user needs to use LAPP for this application.

For ease in doing MEFF calculations, I wrote two short linking programs, MTOB and CONCEN. They enabled automation of MEFF calculations to the maximum extent practicable.

## II. PRELIMINARY THERMOCHEMICAL CALCULATION

Required Results of the Calculation: First of all, one must input appropriate propellant data into a thermodynamics code. The needed output are the quantities required by the interior ballistic code and by MEFF to follow.

Here, IBHVG will be used for the interior ballistic code, so one needs:

Impetus, Adiabatic Flame Temperature, Gamma, and Covolume

For MEFF, one also needs:

Molecular Weight

An Example of the Calculation: The example that has been chosen for this illustrative calculation is for a 155-mm howitzer; and the propellant is the standard M30A1 propellant, which contains 1% (by weight) of  $K_2SO_4$  flash suppressant. A listing of the input job stream and data for this calculation is included as Appendix A.

Note the deliberate suppression of many condensed species, e.g.,  $KCO_2$ ,  $KSO_2$ ,  $K_2O$ , etc., for the calculations. Since the suppressant is presumed to operate in the gas phase, solid-phase or liquid-phase final constituents that could conceivably tie up some of the potassium were not permitted to be formed in these calculations.

The line which begins with CM2 is the listing of the propellant constituents and the weight percentage of each in the propellant:

NC1260	nitrocellulose, 12.60%	27.90% of the total
NG	nitroglycerin	22.42%
NQ	nitroguanidine	46.84%
EC	ethyl centralite	1.49%
KS	potassium sulfate	1.00%

---

5. P. G. Baer and J. M. Frankle, "The Simulation of Interior Ballistic Performance of Guns by Digital Computer Program," BRL Report No. 1183, U.S. Army Aberdeen Research and Development Center, Ballistic Research Laboratories, Aberdeen Proving Ground, MD, December 1962 (AD 299 980).

ALC	ethyl alcohol	0.25%
C	carbon (graphite)	0.01%

In this case, a GUN calculation is desired, with the standard loading density of 0.2 g/cc.

The results of this calculation are shown in detail in Appendix B. The parameter values which carry over directly to the interior ballistic code are:

Impetus	356461 ft-lb/lb
Flame Temperature	3003 K
Gamma	1.2412
Covolume	28.81 in <sup>3</sup>

The values needed for MEFF are:

Molecular Weight	23.432
Covolume	1.041 cc/g

### III. INTERIOR BALLISTIC CALCULATION

Input and Output for the Calculation Next, one must use an interior ballistic code. The input parameters needed are:

Chamber volume, length of travel, propellant mass, projectile mass, and barrel cross section

The output quantities muzzle velocity and mean gas temperature at shot ejection are needed by MEFF, as are several of the gun parameters.

An Example of the Calculation: Appendix C is an IBHVG calculation for the example system. System, projectile, and propellant parameters are nominal values for this system. Note the thermodynamic values introduced from the prior BLAKE calculation.

The results of the interior ballistic calculation needed for MEFF are:

Muzzle velocity	2650 ft/s
Mean gas temp	1860 K

### IV. MEFF CALCULATION

At last one comes to the actual calculation with MEFF itself. The input needed are illustrated by the data on the bottom of the FLASH job stream included as Appendix D. The MEFF listing itself, as modified slightly for automated running, is included as Appendix E. MEFF requirements are as follows:

Data Card	Requirement	Illustrative value
1	A title card	155-MM HOWITZER WITH M203 CHARGE
2	Muzzle velocity	789 m/s
2	Chamber volume	.01966 m <sup>3</sup>
2	Travel	5.08 m

2	Propellant mass	12.23 kg (total of all)
2	Projectile mass	46.36 kg
2	Bore cross section	.0192 m <sup>2</sup>
2	Gamma	1.243
2	Molecular Weight	23.43
2	Mean gas temperature at shot ejection	1861 K
2	Covolume	.001046 m <sup>3</sup> /kg
3	No. iterations between stored values	4
3	Step size	.001
3	Init. condition step away from tau=0	.01
4	Maximum distance from muzzle for calcula- tion to proceed	50. (meters. 10 meters would be appropriate for a mortar calculation.)
4	Print step	5. (meters)
4	Diffusion step size passed to LAPP	.2
4	LAPP output parameter =1, all output =0, centerline temperatures only	1

I have never changed the value of the parameters on the third data card. I added the fourth card so it would be easy to vary the weapon-dependent maximum distance from the muzzle for the calculations, the print step, and the diffusion step size. The fourth parameter on the card makes it easy to reduce the voluminous LAPP output to just centerline temperatures, for troubleshooting. The diffusion step size can be increased, and the run time will be shorter. When one increases the diffusion step size too far, the program will gracefully halt at the moment of ignition. Too large a diffusion step size will not lead to improper results of these calculations.

The output parameters passed from MEFF for calculations to follow are written to TAPE9 at statement 5011, and they are as follows:

TN, the gas temperature at the normal shock when the velocity of the muzzle gas flow becomes sonic

TM0, the muzzle gas temperature at the time of shot ejection

TB, the gas temperature at the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

PM0, the muzzle gas pressure at the time of shot ejection

UB, the gas velocity at the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

ALPHA1, the fraction of gas entering the reflected shock

RB, the radius of the mixing region boundary when the velocity of the muzzle gas flow becomes sonic

XMAX, the maximum distance from the muzzle for the calculations, in meters

PRNT, the print step, in meters

FDL, the diffusion step size, passed through for LAPP

KEY, the LAPP output parameter, passed through for LAPP

## V. MTOB CALCULATION

Next one prepares for thermodynamic calculations at several different places in muzzle exit gas flow space. MTOB (Appendix F) was written to do this automatically. It takes the MEFF output, combines it with the details of the propellant contained in BOIL (Appendix G), and produces TAPE8, which is a detailed command stream for BLAKE and data for programs CONCEN and LAPP to follow.

## VI. BLAKE CALCULATION

Here one needs two thermodynamic calculations, one to calculate the mole fractions at the normal shock, and one to calculate the mole fractions at the reflected shock. The first of these is simply a "point" calculation at the pressure and temperature of the normal shock. For the second, one recalls<sup>1</sup> that the propellant gas expands isotropically from the muzzle to the reflected shock region, so that the mole fractions are the same as those at the muzzle; one thus does a "point" calculation at the pressure and temperature of the muzzle gas as it emerges from the gun.

## VII. CONCEN CALCULATION

The program CONCEN (Appendix H) reads the BLAKE output and automatically calculates the mole fraction for each gaseous species at the initial boundary, as shown in Reference 1.

$$x_i = (1 - \alpha) x_n + \alpha x_r, \text{ where}$$

$x_i$  is the mole fraction at the initial boundary,

$x_n$  is the mole fraction at the normal shock,

$x_r$  is the mole fraction at the reflected shock, and

$\alpha$  is the fraction of the flow that enters the reflected shock.

Thus, the output of CONCEN or of a calculation by some other means, is a list of the 13 gaseous species that LAPP will consider, and the mole fraction of each, in the exact order that LAPP expects to find them:  $H_2O$ ,  $CO$ ,  $H_2$ ,  $N_2$ ,  $CO_2$ ,  $H$ ,  $OH$ ,  $O$ ,  $O_2$ ,  $K$ ,  $KOH$ ,  $KO_2$ ,  $HO_2$ . These results are passed to LAPP on TAPE2.

## VIII. LASTDA, THE LAPP STANDARD DATA SET

The file LASTDA contains the standard LAPP input data, including thermodynamic information on the gaseous species allowed and reaction rate data on the reactions considered. The LAPP report<sup>2</sup> documents the needed LAPP input data in detail; here we concentrate on much-used or often-changed data and on changes from the LAPP report. I have used numbers composed of all 9's to "hold the place" of values which will be replaced in a subsequent read, in order to minimize rewriting LAPP.

LAPP Input Card	Source of input	Via	Input
1	FLASH	TAPE8	Title Card
On card 2, all data entered in I5			
2	LASTDA		Initial number of grid points
2	LASTDA		Number of species (24 max); here 13
2	LASTDA		Viscosity option key; 6=Donaldson/Gray
2	LASTDA		Number of reactions; here 25; LAPP has been modified to handle up through 49
2	LASTDA		Three items specifying output options; all 0
2	LASTDA		Max computer time; never used; here left at 200
2	LASTDA		Pressure option; never changed; here 0
2	LASTDA		Number of thermo entries for each species; here 22 and never changed
3	LASTDA		Signal frequencies; left blank since no attenuation calculations are desired
On card 4, all data entered in E10.3			
4	LASTDA		Initial value of X, the distance from the muzzle, in meters.
4	FLASH	TAPE8	Final value of X in meters.
4	FLASH	TAPE8	Print increment in meters
4	LASTDA		Lewis number, here always 1
4	LASTDA		Prandtl number, here always 1
4	MEFF	TAPE8	Initial Boundary Radius, in meters
4	LASTDA		Factor used to vary eddy viscosity, here always 1
On card 5, all data entered in E10.3			
5	LASTDA		Minimum integration step size, here always .1E-10
5	FLASH	TAPE8	Diffusion step size, FDL
5	LASTDA		Pressure coefficients, here always zero
On card 6, all data entered in E10.3			
6	LASTDA		Pressure at initial value of X, in atmospheres, here always 1
6	MEFF	TAPE8	Temperature at initial boundary in K
6	LASTDA		Ambient air temperature in K, here always 294
6	MEFF	TAPE8	Gas velocity at the initial boundary, in m/s
6	LASTDA		Ambient air velocity in m/s, here always 3.0. Should never be set to 0.
6	LASTDA		$\Psi$ . Here always blank, so program calculates this quantity.
6	LASTDA		Kinetics cut-off temperature in K, here always 200
7			
8	LASTDA		Mole fractions of the allowed gaseous species
9			in the ambient air

10  
 11           CONCEN     TAPE2     Mole fractions of the allowed gaseous species  
 12                                   at the initial boundary

Next in LASTDA come the thermodynamic data on the allowed gaseous species, in JANAF-table format.<sup>6</sup> These are only changed when new data are published. Each species name is entered in A6 format, and all data are then entered in E10.3 format. The ordering of the species in this table determines the order in which LAPP processes the species in all of its transactions. It even specifies which species to associate with the initial number densities which have already been read in from this data set.

Last in LASTDA are the reaction-rate data for the 25 reactions. The reactions may be listed in any order. The data for the C-N-O-H and K reactions have been fairly thoroughly used and checked. At the time this report is written, they are the best available set of reactions and the best available reaction rates for those reactions; but they are not represented here as being the final correct description for the reactions.

The format for each reaction follows:

Column	Item	Format
1-6	Species A	A6
7	+ sign	
8-13	Species B (or M)	A6
14	+ sign (if needed)	
15-20	Blank or M	
21	= sign	
22-27	Species C	A6
28	+ sign (if needed)	
29-34	Species D (or M)	A6
35	+ sign (if needed)	
36-41	Species E (or M)	A6
42-48	Blank	
49-50	Reaction type, 1 to 10 (see below)	I2
51	Rate coefficient type, 1 to 7 (see below)	I1
52-59	A, Pre-exponential factor, cm-molecule-sec units	E8.2
60-63	N, Temperature exponent	F4.1
64-72	B, Activation energy, cal/mole	F9.1

The ten possible reaction types are these:

1	A + B	↔	C + D
2	A + B + M	↔	C + M
3	A + B	↔	C + D + E
4	A + B	↔	C
5	A + M	↔	C + D + M
6	A + B	→	C + D
7	A + B + M	→	C + M
8	A + B	→	C + D + E

6. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables, SECOND EDITION," Dow Chemical Company, Midland, MI, July 1970.

9     A + B     → C  
 10    A + M     → C + D + M

The seven possible rate coefficient types are these:

- 1      $k = A$
- 2      $k = AT^{-1}$
- 3      $k = AT^{-2}$
- 4      $k = AT^{-\frac{1}{2}}$
- 5      $k = A \exp(B/RT)$
- 6      $k = AT^{-N} \exp(B/RT)$
- 7      $k = AT^{-\frac{3}{2}}$

## X. FINAL RESULTS

Some of the pages of the final results of the illustrative calculation are included as Appendix K. The total calculation took 78 CPU seconds on MFZ, all but 14.5 seconds of which was LAPP execution.

MEFF results are followed by BLAKE calculations at the two necessary combinations of temperature and pressure. These are followed by the results of CONCEN, the combined mole fractions at the initial boundary.

Finally come the results of the LAPP calculation. First the input parameters are echoed. Then, at each desired distance from the muzzle, as a function of the distance from the centerline of the flight of the projectile, there are gas temperature, velocity, density, etc. and mole fractions for each of the allowed gaseous constituents. Included in Appendix K are the prints for the flow from the muzzle ( $X = 0$  meters), for  $X = 10$  meters (where one notes a maximum gas temperature of 1079 K), for  $X = 15.3$  meters, and for  $X = 42$  m. The prints at 15.3 meters are the most interesting, for they show that the maximum temperature has risen to 2018 K, indicating that ignition has taken place. If there had been sufficient suppressant to eliminate the flash, one would have seen the temperature rise to 1100 K or 1200 K and then decline slowly, indicating that the mixture had cooled before ignition could take place.

It was noted earlier that one could set  $KEY = 0$  in the input job stream for MEFF/LAPP (Appendix D), and that then one would have gotten only the centerline temperatures from LAPP. Notice that even then, by 42 meters the centerline temperature has exceeded 2000 K, so that even with a limited print, ignition is unmistakably indicated.

#### ACKNOWLEDGMENTS

I especially appreciate all of those whose desire to make flash prediction calculations with MEFF and LAPP encouraged me to write this users' guide. They include, but are not limited to, W. Lippincott, P. Baer, T. Coffee, and A. Bracuti.

## REFERENCES

1. V. Yousefian, "Muzzle Flash Onset," ARI-RR-236, Aerodyne Research, Inc., Billerica, MA, November 1980. Also available as ARBRL-CR-00477, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD February 1982 (AD B063 573L).
2. R. R. Mikatarian, C. J. Kau, and H. S. Pergament, "A Fast Computer Program for Nonequilibrium Rocket Plume Predictions," AFRPL-TR-72-94, Air Force Rocket Propulsion Laboratory, Edwards Air Force Base, CA, August 1972.
3. J. Corner, Theory of Interior Ballistics of Guns, John Wiley & Sons, New York (1950).
4. E. Freedman, "BLAKE - A Thermodynamic Code Based on TIGER: User's Guide and Manual," ARBRL-TR-02411, USA ARRADCOM, Ballistic Research Laboratory, Aberdeen Proving Ground, MD, July 1982 (AD A121 259).
5. P. G. Baer and J. M. Frankle, "The Simulation of Interior Ballistic Performance of Guns by Digital Computer Program," BRL Report No. 1183, U.S. Army Aberdeen Research and Development Center, Ballistic Research Laboratories, Aberdeen Proving Ground, MD, December 1962 (AD 299 980).
6. D. R. Stull and H. Prophet, "JANAF Thermochemical Tables, SECOND EDITION," Dow Chemical Company, Midland, MI, July 1970.

APPENDIX A

BLA30A1, INPUT FOR A BLAKE CALCULATION

GEK,STMFZ,P6,T120.BLA30A1  
ACCOUNT,XXXXXX.  
ATTACH,TT,BLAKELIBRARY,ID=ELI.  
COPY,TT,TAPE7.  
RETURN,TT.  
REWIND,TAPE7.  
ATTACH,B,BLAKE,ID=ELI.  
B.  
EXIT.  
\*EOR  
TIT,M30A1  
PRL,CON,2  
REJ,N,K2SO4,C,C2,CH,CH2O,HNO3  
REJ,C(S),K2SO4\$  
REJ,KOH\$,KO2\$,K2O2\$  
REJ,H2S,S2O,S02,K\$,K2O,K2O2  
REJ,KCO\$,KSO\$,K2O\$,K\$  
REJ,K2CO3\$  
REJ,K2S\$  
UNI,ENG  
CM2,NC1260,27.9,NG,22.42,NQ,46.84,EC,1.49,KS,1.,  
ALC,.25,C,.1  
GUN,.1,.1,.5  
QUIT

APPENDIX B  
BLAKE CALCULATION

M30A1

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1260	27.900	.018	-1.6916E+08	C 6000 H 7549 O 9901 N 2451
NG	22.420	17.201	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	46.840	78.418	-2.2100E+04	C 1 H 4 O 2 N 4
EC	1.490	.967	-2.5100E+04	C 17 H 20 O 1 N 2
KS	1.000	1.000	-3.4266E+05	K 2 S 1 O 4
ALC	.250	.945	-6.6420E+04	C 2 H 6 O 1
C	.100	1.451	0.	C 1

THE HEAT OF FORMATION IS -384.86 CAL/GRAM = -6.7053E+04 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	14.896
H	32.439
O	28.660
N	23.830
K	.116
S	.058

M30A1

THERE ARE 29 GASEOUS CONSTITUENTS SELECTED

NAME	BKW	L-J	EPS/K	L-J	SIGMA	A1	A2	A3	T H E R M O				C O N S T A N T S				A6	A7	A8	A9
1. CO	390.0	91.7	3.690	3.690	5.83775	5.83775	-.40270	.06491	-.00373	-.00373	-.00373	-.00373	-2.14066	.71717	.71717	.71717	-.08241	-.08241	-31130.5	53.1746
2. H2O	250.0	542.5	2.790	2.790	7.60069	7.60069	.39388	-.10260	.00807	.00807	.00807	.00807	-4.86836	2.30899	2.30899	2.30899	-.37689	-.37689	-62860.1	47.1008
3. CO2	600.0	195.2	3.941	3.941	9.06744	9.06744	-.40694	.06138	-.00273	-.00273	-.00273	-.00273	-2.70529	.56199	.56199	.56199	-.04428	-.04428	-102647.7	60.2574
4. N2	380.0	71.4	3.798	3.798	5.90618	5.90618	-.39603	.05863	-.00307	-.00307	-.00307	-.00307	-2.41322	.89566	.89566	.89566	-.11540	-.11540	-4589.1	51.2455
5. H2	180.0	59.7	2.827	2.827	4.48064	4.48064	.19824	-.00851	-.00003	-.00003	-.00003	-.00003	-1.97442	1.15151	1.15151	1.15151	-.21216	-.21216	-2116.7	36.2744
6. NO	386.0	116.7	3.492	3.492	5.77838	5.77838	-.43892	.08202	-.00561	-.00561	-.00561	-.00561	-1.79245	.50895	.50895	.50895	-.04564	-.04564	16765.3	57.0969
7. KOH	0.0	100.0	3.500	3.500	7.27052	7.27052	.40176	-.10705	.00896	.00896	.00896	.00896	-1.70167	.87842	.87842	.87842	-.16291	-.16291	-59999.7	68.1294
8. NH3	476.0	558.3	2.900	2.900	13.60629	13.60629	-.93312	.18185	-.00958	-.00958	-.00958	-.00958	-9.06058	3.51672	3.51672	3.51672	-.50840	-.50840	-22985.7	45.5074
9. HCN	359.0	344.7	3.339	3.339	9.48792	9.48792	-.37342	.04424	-.00222	-.00222	-.00222	-.00222	-4.59416	1.73907	1.73907	1.73907	-.25679	-.25679	24383.5	53.6459
10. CH4	528.0	148.6	3.758	3.758	20.35251	20.35251	-.1.95871	.26284	-.01397	-.01397	-.01397	-.01397	-14.43248	5.11197	5.11197	5.11197	-.67906	-.67906	-38010.8	38.5449
11. COS	0.0	100.0	3.500	3.500	9.07572	9.07572	-.4.7894	.09730	-.00658	-.00658	-.00658	-.00658	-2.27231	.48548	.48548	.48548	-.04719	-.04719	-41172.7	66.5255
12. C2H4	372.0	224.7	4.163	4.163	22.63477	22.63477	-.1.64131	.20002	-.00937	-.00937	-.00937	-.00937	-13.78191	4.49325	4.49325	4.49325	-.59268	-.59268	-10548.7	51.3360
13. C2H2	0.0	100.0	3.500	3.500	12.54085	12.54085	-.1.6675	.02155	-.00023	-.00023	-.00023	-.00023	-5.90900	2.01409	2.01409	2.01409	-.26643	-.26643	43014.0	54.7220
14. O2	350.0	106.7	3.467	3.467	2.20306	2.20306	.1.12042	-.18485	.01276	.01276	.01276	.01276	2.02364	-1.20737	-1.20737	-1.20737	.22334	.22334	-2085.5	59.2300
15. K	0.0	100.0	3.500	3.500	6.09867	6.09867	-.1.44727	.10388	-.03850	-.03850	-.03850	-.03850	-3.46738	1.37555	1.37555	1.37555	-.18637	-.18637	16559.0	41.4178
16. S	0.0	100.0	3.500	3.500	1.83331	1.83331	.19365	.01065	-.00358	-.00358	-.00358	-.00358	.77619	-1.26477	-1.26477	-1.26477	.03824	.03824	65713.8	47.5476
17. C2N2	0.0	100.0	3.500	3.500	13.82927	13.82927	-.1.13108	.19089	-.01258	-.01258	-.01258	-.01258	-5.06809	1.56648	1.56648	1.56648	-.19796	-.19796	61813.4	70.4037
18. OH	226.0	100.0	3.500	3.500	4.22400	4.22400	.47240	-.11211	.00942	.00942	.00942	.00942	-1.70189	.97134	.97134	.97134	-.16944	-.16944	7437.0	49.0478
19. KO	0.0	100.0	3.500	3.500	4.49837	4.49837	.11393	.00019	-.00002	-.00002	-.00002	-.00002	.00503	-.02588	-.02588	-.02588	.00186	.00186	14185.2	67.4039
20. SO	0.0	100.0	3.500	3.500	1.92172	1.92172	1.33802	-.22714	.01363	.01363	.01363	.01363	2.24044	-1.13902	-1.13902	-1.13902	.18518	.18518	-219.7	63.6970
21. S2	0.0	100.0	3.500	3.500	4.48800	4.48800	.03544	-.00050	.00003	.00003	.00003	.00003	.02430	-.11854	-.11854	-.11854	.01769	.01769	27643.9	64.5607
22. HS	0.0	100.0	3.500	3.500	6.12907	6.12907	-.41325	.06726	-.00371	-.00371	-.00371	-.00371	-2.95581	1.32672	1.32672	1.32672	-.19604	-.19604	30547.3	51.9361
23. CH3	525.0	100.0	3.500	3.500	13.82287	13.82287	-.74765	.05695	-.00032	-.00032	-.00032	-.00032	-9.14376	3.65133	3.65133	3.65133	-.54025	-.54025	23004.1	46.4265
24. H	13.4	100.0	3.500	3.500	2.49993	2.49993	.00000	-.00000	.00000	.00000	.00000	.00000	.00000	-.00000	-.00000	-.00000	.00000	.00000	50621.8	33.4041
25. O	212.8	100.0	3.500	3.500	2.97972	2.97972	-.25641	.05953	-.00389	-.00389	-.00389	-.00389	-.43119	1.19753	1.19753	1.19753	-.02943	-.02943	57760.7	44.3789
26. CHD	700.0	100.0	3.500	3.500	10.04357	10.04357	-.1.09647	.20969	-.01480	-.01480	-.01480	-.01480	-6.57561	1.36019	1.36019	1.36019	-.14753	-.14753	955.9	59.4686
27. CH2	525.0	100.0	3.500	3.500	11.42150	11.42150	-.1.32276	.21610	-.01403	-.01403	-.01403	-.01403	-7.38097	3.01187	3.01187	3.01187	-.44496	-.44496	83047.1	47.9048
28. CN	0.0	100.0	3.500	3.500	2.71179	2.71179	.54169	.09568	-.02040	-.02040	-.02040	-.02040	1.50282	-1.01851	-1.01851	-1.01851	.20537	.20537	101465.0	58.3631
29. K2	0.0	100.0	3.500	3.500	4.50198	4.50198	.24737	.00004	.00000	.00000	.00000	.00000	-.00245	-.00020	-.00020	-.00020	-.00023	-.00023	27675.0	70.3214

THE FLOOR IS AT 14

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TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	1)	2)	3)
N2	1.17835E+01	1.17756E+01	1.17633E+01
CO	1.16845E+01	1.17189E+01	1.17434E+01
H2O	1.04224E+01	1.04928E+01	1.05490E+01
H2	5.49904E+00	5.42160E+00	5.33950E+00
CO2	3.04189E+00	2.99399E+00	2.95515E+00
KOH	1.02155E-01	1.06154E-01	1.08132E-01
COS	1.24913E-02	1.97122E-02	2.57452E-02
NH3	9.60859E-03	2.35990E-02	4.35205E-02
NO	6.45435E-03	4.35300E-03	3.34043E-03
HCN	2.72481E-03	7.11492E-03	1.39539E-02
O2	2.42410E-04	1.03891E-04	5.79830E-05
CH4	8.74142E-03	4.65937E-04	1.40821E-03
C2H2	1.10729E-06	6.86994E-06	2.40198E-05
C2H4	2.48644E-08	3.29884E-07	1.86232E-06
K	1.024966E-02	0.52656E-03	6.57183E-03
S	1.96564E-03	1.24340E-03	8.54751E-04
C2N2	2.72369E-08	1.91412E-07	7.57681E-07
OH	3.90690E-02	2.46999E-02	1.77802E-02
KO	1.14157E-04	8.08104E-05	5.96825E-03
SO	1.37149E-02	8.67324E-03	1.48727E-03
S2	1.81570E-03	1.72835E-03	2.18473E-02
HS	2.58660E-02	2.43007E-02	2.09539E-04
CH3	2.38197E-05	8.77368E-05	2.86234E-02
H	6.42166E-02	4.01198E-02	5.99457E-05
D	2.96179E-04	1.26139E-04	4.09603E-03
CHO	1.83960E-03	2.95975E-03	2.80760E-06
CH2	6.12020E-07	1.52314E-05	1.11839E-05
CN	4.36160E-06	7.55025E-06	6.34867E-06
K2	4.83636E-06	5.66071E-06	42.6341
TOTAL GAS (MOLES/KG)	42.7266	42.6770	42.6341

\*\* PROGRAM BLAKE, VERSION 205.11 \*\*

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\*\* SUMMARY OF PROPELLANT THERMO PROPERTIES \*\*

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

RHO/L G/CC	TEMP K	PRESSURE MPA	IMPETUS J/G	MOL WT GAS	CO-VOL CC/G	FROZEN GAMMA	CP(FR)	B(T) CC	C(T) CH#6	GAS VOL CC/G	S J/G-K	H J/G	E J/G	ADEXP	PHI
1)	.1000	2992.	119.22	1062.9	1.084	1.2380	43.77	26.09	555.	10.000	9.57	-418.2	-1610.3	1.3738	1.1216
2)	.2000	3003.	269.13	1065.3	1.041	1.2412	44.20	26.08	555.	5.000	9.29	-264.6	-1610.2	1.5338	1.2629
3)	.3000	3010.	455.81	1066.9	.993	1.2471	44.73	26.06	555.	3.333	9.12	-90.9	-1610.2	1.6953	1.4241

  

RHO/L G/CC	TEMP K	PRESSURE PSI	IMPETUS FT-LB/LR	MOL WT GAS	CO-VOL CU IN	FROZEN GAMMA	CP(FR)	B(T) CU IN	C(T) IN#6	GAS VOL CU IN/LB	S GIBBS	H CAL/MOL	E CAL/MOL	ADEXP	PHI
1)	.1000	2992.	17291.	355609.	30.01	1.2380	10.46	1.592	2.07	276.799	2.29	-99.9	-384.9	1.3738	1.1216
2)	.2000	3003.	39034.	356461.	28.81	1.2412	10.56	1.591	2.07	138.399	2.22	-63.2	-384.9	1.5338	1.2629
3)	.3000	3010.	66110.	356933.	27.48	1.2471	10.69	1.590	2.06	92.266	2.18	-21.7	-384.9	1.6953	1.4241

APPENDIX C  
IBHVG CALCULATION

GUN TYPE: 155-MM HOWITZER  
 CHAMBER VOLUME: 1200.00 CU IN  
 GROOVE DIAMETER: 6.200 IN  
 GROOVE/LAND RATIO: 1.660  
 TWIST: ONE TURN IN 20.0 CALIBERS  
 PRESSURE GRADIENT: LAGRANGIAN  
 PROJECTILE: M483A1

BORE LENGTH: 200.0 IN  
 TIME STEP: .100 MS  
 LAND DIAMETER: 6.100 IN  
 BORE AREA: 29.828 SQ IN  
 EXPANSION RATIO: 6.0  
 EROSION COEFF: .0000500  
 PROJ WT: 102.200 LB

# ENGRAVING & FRICTIONAL RESISTANCE [KPSI] VS. TRAVEL [IN]:

TRAVEL:	0.00	.40	1.00	1.55	2.05	4.50	200.00
RESISTANCE:	.25	3.35	4.95	3.63	3.25	2.80	1.50

PROPELLANT	BLK POWDR	M30A1	NC TUBE
WEIGHT [LB]	.315	26.150	.500
IMPETUS [FT-LB/LB]	96000.	356461.	180000.
FLAME TEMP [K]	2000.	3003.	1553.
ALPHA	0.0000	.7000	0.0000
BETA	50.000000	.003950	30.000000
GAMMA	1.250	1.241	1.250
COVOL [CU IN/LB]	30.000	28.810	30.000
DENS [LB/CU IN]	.06000	.05717	.03400
GRAIN TYPE	CORD	7-PERF	SHEET
GRAIN LEN [IN]	.2000	.9481	28.0000
GRAIN WIDTH [IN]	-----	-----	1.5000
GRAIN DIAM [IN]	.1000	.4173	-----
PERF DIAM [IN]	-----	.0338	-----
GRAIN THICK [IN]	-----	-----	.1250
INNER WEB [IN]	-----	.0790	-----
OUTER WEB [IN]	-----	.0790	-----
IGNITION CODE	0	0	0
THRESHOLD VALUE	0.00000	0.00000	0.00000

# STDM203, A STANDARD M203 CHARGE IN A 155-MM HOWITZER

CONDITIONS AT:	MAX PR	MUZZLE	PROP 1	PROP 2	PROP 3
			BURNT	BURNT	BURNT
TIME [MS]	6.65	13.69	1.00	11.20	2.10
BR PRES [KPSI]	47.77	11.48	3.01	19.96	9.04
MN PRES [KPSI]	46.02	11.10	2.91	19.26	8.81
BS PRES [KPSI]	42.52	10.34	2.72	17.88	8.35
MEAN TEMP [K]	2622.	1860.	2266.	2088.	2530.
TRAVEL [IN]	23.9	200.0	.0	124.4	.4
VEL [FPS]	1104.	2650.	9.	2377.	48.
ACCEL [G'S]	11615.	2530.	644.	4593.	1524.
FR BRNT PROP 1	1.000	1.000	1.000	1.000	1.000
FR BRNT PROP 2	.571	1.000	.010	1.000	.043
FR BRNT PROP 3	1.000	1.000	.502	1.000	1.000

## APPENDIX D

FLASH, THE JCL AND INPUT DATA FOR MEFF, MTOB, BLAKE, CONCEN, AND LAPP

GEK, STMFZ, P1, T300.FLASH  
 ACCOUNT, XXXXXXXX.  
 BEGIN, GETMFA, FILE, LF=A, PF=MEFF, UN=GEK. CREATES TAPE9  
 MAP, OFF.  
 FTN, I=A, L=0, R=0, T.  
 LGO.  
 REWIND, TAPE9.  
 BEGIN, GETMFA, FILE, LF=E, PF=MTOB, UN=GEK.  
 BEGIN, GETMFA, FILE, LF=TAPE4, PF=BOIL, UN=GEK. BLAKE BOILERPLATE  
 FTN, B=LGO3, I=E, L=0, R=0, T.  
 LGO3.  
 REWIND, OUTPUT.  
 COPY, OUTPUT, TAPE8.  
 REWIND, TAPE8. FILE OF BLAKE, CONCEN, AND LAPP DATA  
 ATTACH, TT, BLAKELIBRARY, ID=ELI.  
 COPY, TT, TAPE7.  
 RETURN, TT.  
 REWIND, TAPE7.  
 ATTACH, B, BLAKE, ID=ELI.  
 B, TAPE8.  
 REWIND, OUTPUT.  
 REWIND, TAPE1.  
 COPY, OUTPUT, TAPE1.  
 REWIND, TAPE1. INPUT FOR CONCEN  
 BEGIN, GETMFA, FILE, LF=C, PF=CONCEN, UN=GEK.  
 FTN, B=LGO1, I=C, L=0, R=0, T.  
 LGO1.  
 REWIND, TAPE2.  
 BEGIN, GETMFA, FILE, LF=TAPE3, PF=LASTDA, UN=GEK.  
 REWIND, TAPE3.  
 BEGIN, GETMFA, FILE, LF=D, PF=LAPP, UN=GEK.  
 FTN, B=LGO2, I=D, L=0, R=0, T.  
 LGO2.  
 EXIT.  
 155-MM HOWITZER WITH M203 CHARGE  
 807.7, .019664, 5.08, 12.23, 46.36, .019244, 1.241, 23.432, 1860., .001041  
 4, .001, .01  
 50., 5.0, 0.20, 1

APPENDIX E  
MEFF PROGRAM LISTING

```

      PROGRAM MEFF(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT,TAPE9)
C
C MAIN: MUZZLE FLASH
C
C MUZZLE PROPERTIES VS TIME
C
C TYPE DATA CARDS USING NAMELIST FORMAT
C
C   TITLE CARD FIRST
C
C   *PHYSIC*
C       V0=MUZZLE VELOCITY(M/SEC)
C       L=BORE LENGTH(M)
C       MP=MASS OF PROPELLANT
C       W=MASS OF PROJECTILE(KG)
C       A=CROSS SECTIONAL AREA OF BORE(M**2)
C       GAM=RATIO SPECIFIC HEATS PROPELLANT GAS
C       MBAR=MEAN MOL WEIGHT PROPELLANT
C       TF=FLAME TEMPERATURE(K)
C       TA=AVERAGE BARREL GAS TEMPERATURE(K)
C       CVO=CHAMBER VOLUME(M**3)
C       ETA=COVOLUME FOR VAN DER WAAL'S EQ. STATE(M**3/KG)
C
C   *MATH*
C       M=NUMBER OF ITERATIONS BETWEEN STORED VALUES
C       DELTAU=STEP SIZE
C       DLTAU0=INITIAL CONDITION STEP AWAY FROM TAU=0
C
      REAL MP,L,MBAR,LAMM,M0,MACHNO,MR,MNP2
      COMMON/WORKA/LAMM,GAM,EPS,M0,B0,C0,D0,KPMAX
      COMMON/WORKB/THETA(500),Z(500),H1(500),H1P(500),THETAP(500),
1 TTAU(500),FEJECT(500)
      COMMON/WORKC/TEFF,ETA,A,L,MP,V0,ALMP,R
      COMMON/WORKD/PE(50),UE(50),TE(50),RHOE(50),TIME(50),
1 TEMP(50),FKP(50),CO2(50),CO(50),H2O(50),H2(50)
      DIMENSION TITLE(20)
      NAMELIST/PHYSIC/V0,L,MP,W,A,GAM,MBAR,TF,TA,ETA,CVO
      NAMELIST/MATH/M,DELTAU,DLTAU0
      DATA IREAD,IWRITE/5,6/
      DATA IMAX/500/,IZTHET/0/,PI/3.141592654/
C
C READ IN DATA
C
      READ(IREAD,1111)TITLE
      1111 FORMAT(20A4)
      WRITE(9,1111)TITLE
      1000 FORMAT(1H1,20A4)
      READ(IREAD,*)V0,CVO,L,MP,W,A,GAM,MBAR,TA,ETA
C   CALL NMLST('PHYSIC',0,5,V0,L,MP,W,A,GAM,MBAR,TF,TA,ETA,CVO)
      READ(IREAD,*)M,DELTAU,DLTAU0
C   CALL NMLST('MATH ',0,5,M,DELTAU,DLTAU0)
C
C READ MAX DIST, PRINT STEP, DIFFUSION STEP SIZE, AND KEY; ALL FOR LAPP.
C KEY=1 FOR ALL LAPP PRINTS, =0 FOR CENTERLINE ONLY.
C
      READ(IREAD,*)XMAX,PRNT,FDL,KEY

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C      CALBER = 1000. * SQRT( 4.*A/3.141593 )
C
      IF(TF.EQ.0.0) GO TO 1
      WRITE(IWRITE,1000) TITLE
      WRITE(IWRITE,1010) V0,L,MP,W,CALBER,A,GAM,MBAR,TF,ETA,
1CVO
1010 FORMAT('0',' MUZZLE VELOCITY V0 =',G10.4,' M/SEC'/
1' ',' BORE LENGTH L =',G10.4,' METERS'/
2' ',' PROPELLANT MASS MP =',G10.4,' KG'/
3' ',' PROJECTILE MASS W =',G10.4,' KG'/
4' ',' GUN CALIBER CALBER =',G10.4,' MM'/
5' ',' BARREL CROSS SECTIONAL AREA A =',G10.4,' M**2'/
6' ',' SPECIFIC HEAT RATIO OF PROPELLANT GAS GAM =',G10.4/
7' ',' MEAN MOLECULAR WEIGHT OF PROPELLANT GAS MBAR =',G10.4,
8 /
9' ',' FLAME TEMPERATURE TF =',G10.4,' DEG K'/
1' ',' COVOLUME ETA =',G10.4,' M**3/KG'/
2' ',' CHAMBER VOLUME CVO =',G10.4,' M**3'/)
      WRITE(6,6001)
      GO TO 6000
1  WRITE(IWRITE,1000) TITLE
      WRITE(IWRITE,1110) V0,L,MP,W,CALBER,A,GAM,MBAR,TA,ETA,
1 CVO
1110 FORMAT('0',' MUZZLE VELOCITY V0 =',G10.4,' M/SEC'/
1' ',' BORE LENGTH L =',G10.4,' METERS'/
2' ',' PROPELLANT MASS MP =',G10.4,' KG'/
3' ',' PROJECTILE MASS W =',G10.4,' KG'/
4' ',' GUN CALIBER CALBER =',G10.4,' MM'/
5' ',' BARREL CROSS SECTIONAL AREA A =',G10.4,' M**2'/
6' ',' SPECIFIC HEAT RATIO OF PROPELLANT GAS GAM =',G10.4/
7' ',' MEAN MOLECULAR WEIGHT OF PROPELLANT GAS MBAR =',G10.4,
8 /
9' ',' AVERAGE BARREL GAS TEMPERATURE TA =',G10.4,' DEG K'/
1' ',' COVOLUME ETA =',G10.4,' M**3/KG'/
2' ',' CHAMBER VOLUME CVO =',G10.4,' M**3'/)
      WRITE(6,6001)
6000 CONTINUE
C
C CALCULATED PARAMETERS
C
      L=L+CVO/A
      ALMP = A*L/MP
      LAMM=MP/W
      R=8317./MBAR
      TEFF = TF - .5*(GAM-1.)*V0*V0*(.3333+1./LAMM)/R
      IF(TA.NE.0.0)TEFF=TA
      EPS=ETA/(ALMP-ETA)
      M0=V0/SQRT(GAM*R*TEFF)
C
C
C INITIAL CONDITIONS: THET0
C
      C=1.+EPS
      G10=C+LAMM/(3.*GAM)

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      G10P=G10-LAMM*(C/M0+.5)/GAM
C
      J = 0
      YOLD = (2.-M0+C)/(M0+C)
      EXP = 2./(GAM+1.)
20    J = J + 1
      IF(J.GE.15) GO TO 20
      DENOM = M0 + 1. + EPS + (M0-1.-EPS)/YOLD
      YNEW = (EPS + (2.*G10/DENOM)**EXP) / G10
C
      IF(ABS(YNEW-YOLD).LE..00001) GO TO 30
      YOLD = YNEW
      GO TO 20
C
30    THET0 = YNEW
C
C
C
C INITIAL CONDITIONS: THET0P
C
      ALPHA=.5*(GAM+1.)/(1.-EPS/(THET0*G10))
      BETA=-1.*THET0*(M0+C)/(M0-C)
      BPRIME=-1.+LAMM/(GAM*M0*M0)
      CPRIME=.5*(1.-GAM)-GAM*EPS
      DELTA=(BPRIME*(1.+THET0)+CPRIME*(THET0-1.)/M0)/(1.-C/M0)
      THET0P =THET0*((1.+THET0)*(1.-G10P/G10)+DELTA+
1G10P*(1.-ALPHA)*(BETA-1.)/G10)/(2.+ALPHA*(BETA-1.))
C
C
C SUBROUTINE ZTHETA INTEGRATES DIFFERENTIAL EQ. FOR THETA
C ZTHETA CALLS RUNGE-KUTTA SCHEME SUBROUTINES GILL AND GILL1
C ZTHETA CALLS DERIV TO CALCULATE DERIVATIVES OF Z AND THETA
C
      CALL ZTHETA(DELTAU,DLTAU0,THET0,THET0P,IMAX,M,I,G10,EJECTO)
C
C PRINT MUZZLE PROPERTIES
C
      DO 60 K=1,I
      T=TTAU(K) * L/V0 * 1000.
      RHO2=EPS/(ETA*H1(K))
      V2=SQRT(GAM*R*TEFF)*H1(K)/(H1(K)-EPS)**(.5*(GAM+1.))
      T2=TEFF*(H1(K)-EPS)**(1.-GAM)
      P2=R*T2/(1./RHO2-ETA)
      P2ATM = P2 / 101325.
      SONICV = SQRT( GAM*R*T2 )
      MACHNO = V2 / SONICV
      FEJECT(K) =FEJECT(K)/ M0 / (1.-ETA*MP/(A*L))
      IF(MACHNO.LT.1.0)GO TO 1001
      ZSQ=.476*GAM*P2ATM
      ZSQ1=SQRT(ZSQ)
      XM2=(.4*ZSQ)**(GAM-1.)*(GAM+1.)/((GAM-1.)**GAM)
      DO 2000 J=1,50
      AB=1./(GAM-1.)
      ABC=AB*GAM
      ABCD=(2.+(GAM-1.)*XM2)
      ABCDE=2.*GAM*XM2-(GAM-1.)

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      XFMP=-.49*GAM**2*(1./(GAM+1.))**AB*(ABCD**AB-2.*ABCD**ABC/ABCDE)/
1ABCDE
      XFM=ZSQ-.49*GAM*(1./(GAM+1.))**AB*ABCD**ABC/ABCDE
C      WRITE(1,2001)XFM,XM2
      IF(ABS(XFM).LT..001) GO TO 2002
      XM2=XM2-XFM/XFMP
      IF(J.EQ.50)STOP 10
2000 CONTINUE
2002 XM1=SQRT(XM2)
      PM0=R*TEFF*(1.0-LAMM/3.0)/(ALMP-ETA)
      PM0=PM0/101325.
      TM0=TEFF*(1.0-(GAM-1.0)*LAMM/(GAM*3.0))
      GAMP1=GAM+1.0
      GAMM1=GAM-1.0
      AXX=GAMM1/GAM
      MR=(GAMP1*P2ATM**AXX-2.0)/GAMM1
      MR=SQRT(MR)
      TR=T2*GAMP1/(2.0+GAMM1*MR**2)
      UR=SQRT(GAM*R*TR)*MR
      TN1=GAMP1/(2.0+GAMM1*XM1**2)
      TN2=1.0+2.0*GAMM1*(GAM*XM2+1.0)*(XM2-1.0)/(XM2*GAMP1**2)
      TN=TN1*TN2*T2
      MNP2=(2.0+GAMM1*XM2)/(2.0*GAM*XM2-GAMM1)
      UN=SQRT(MNP2*R*TN*GAM)
      EPSD=.69*SQRT(GAM*P2ATM)
      XXY=GAMP1/(2.0*GAMM1)
      XXY=(GAMP1/(2.0+GAMM1*XM2))**XXY
      TETTA=.96*EPSD**2*XM1*XXY
      UB=(1.0-TETTA)*UR+TETTA*UN
      TB1=(1.0-TETTA)*TETTA*GAMM1/2.0
      TB2=MR**2*(1.0-(UN/UR)**2)*TR
      TB=(1.0-TETTA)*TR+TETTA*TN+TB1*TB2
      PR=1.0
      UMS=SQRT(GAM*R*T2)
      AB=P2ATM*(TB/T2)*(UMS/UB)*A
      RB=SQRT(AB/PI)
      WRITE(6,5000)
5000 FORMAT(32X,48HMUZZLE GAS PROPERTIES WHEN PROJECTILE IS EJECTED,/)
      WRITE(6,6001)
      WRITE(6,5001)PM0
5001 FORMAT(40X,9HPRESSURE=,2X,F7.2,4H ATM)
      WRITE(6,5002)TM0
5002 FORMAT(40X,12HTEMPERATURE=,2X,F7.1,2H K)
      WRITE(6,5003)V0
5003 FORMAT(40X,9HVELOCITY=,2X,F7.1,6H M/SEC)
      WRITE(6,6001)
6001 FORMAT(2X,///)
      WRITE(6,5004)
5004 FORMAT(32X,56HMUZZLE GAS PROPERTIES WHEN MUZZLE VELOCITY BECOMES S
1ONIC,/)
      WRITE(6,6001)
      WRITE(6,5001)P2ATM
      WRITE(6,5002)T2
      WRITE(6,5003)UMS
      FEJ=FEJECT(K)

```

```

        WRITE(6,5005)FEJ
5005  FORMAT(40X,31HFRACTION OF EJECTED PROPELLANT=,2X,F6.4)
        WRITE(6,6001)
        WRITE(6,5006)
5006  FORMAT(32X,69HFLOW CONDITIONS AT REFLECTED SHOCK WHEN MUZZLE VELOC
        1ITY BECOMES SONIC,/)
        WRITE(6,6001)
        WRITE(6,5001)PR
        WRITE(6,5002)TR
        WRITE(6,5003)UR
        ALPH1=1.0-TETTA
        WRITE(6,5007)ALPH1
5007  FORMAT(40X,41HFRACTION OF GAS ENTERING REFLECTED SHOCK=,2X,F6.4)
        WRITE(6,6001)
        WRITE(6,5008)
5008  FORMAT(32X,66HFLOW CONDITIONS AT NORMAL SHOCK WHEN MUZZLE VELOCITY
        1 BECOMES SONIC,/)
        WRITE(6,6001)
        WRITE(6,5001)PR
        WRITE(6,5002)TN
        WRITE(6,5003)UN
        WRITE(6,6001)
        WRITE(6,5009)
5009  FORMAT(32X,76HFLOW CONDITIONS AT MIXING REGION BOUNDARY WHEN MUZZL
        1E VELOCITY BECOMES SONIC,/)
        WRITE(6,6001)
        WRITE(6,5001)PR
        WRITE(6,5002)TB
        WRITE(6,5003)UB
        WRITE(6,5010)RB
5010  FORMAT(40X,17HBOUNDARY RADIUS =,2X,F6.3,' M',////)
C
        WRITE(9,5011)TN,TM0,TB,PM0,UB,ALPH1,RB,XMAX,PRNT,FDL,KEY
5011  FORMAT(10F8.3,I1)
C  THUS IS DATA PASSED ON TO MTOB, BLAKE, CONCEN, AND LAPP
C
5555  FORMAT(1H,"MACH NO IS .GE. 1")
        IF(MACHNO.GE.1.0)WRITE(6,5555)
        IF(MACHNO.GE.1.0)STOP
C
1001  CONTINUE
C
        WRITE(IWRITE,1090) T,RHO2,V2,P2,P2ATM,T2,SONICV,MACHNO,FEJECT(K)
1090  FORMAT(' ',1P9G13.4)
C
        60 CONTINUE
        IF(I.GT.1)STOP
C
C
C  SUBROUTINE RATEAU CALCULATES THE MUZZLE PROPERTIES AFTER
C  THE RAREFRACTION WAVE HITS THE BREECH
C
        WRITE(IWRITE,1100)
1100  FORMAT('0 RAREFRACTION WAVE HAS HIT THE BREECH'//)
        T = TTAU(I)*L/V0*1000.

```

```

      T2 = TEFF*(H1(I)-EPS)**(1.-GAM)
      EJECTO = EJECTO/M0/(1.-ETA*MP/(A*L))
      CALL RATEAU(T,T2,EJECTO,I,JJ)
C
C PLANE A
C
      WRITE(IWRITE,2110)
2110 FORMAT('1',T45,'PLANE A FLOW PROPERTIES'// ' TIME',T10,
1 'DENSITY',T20,'TEMP',T30,'VELOCITY',T43,'XI/D',T50,'SHOCK',
2 T60,'PLANE A',T70,'CO2',T80,'CO',T90,'H2O',T100,'H2'/
3 ' MSEC',T11,'KG/M3',T21,'DEG K',T31,'M/SEC',T50,'LENGTH',
4 T60,'DIAMETER',T70,'MOL/M3',T80,'MOL/M3',T90,'MOL/M3',
5 T100,'MOL/M3'/)
C
      DO 70 I=1,JJ
      P0 = PE(I)*((GAM+1.)*.5)**(GAM/(GAM-1.))
      XID = .69*SQRT(GAM*PE(I))
      XID = XID/(1. + .197*PHI**.65)
      SHOCKL = 1.25*XID
      HAREA = A*SQRT(.5*(GAM-1.))*(2./(GAM+1.))**((GAM+1.)*.5/
1 (GAM-1.))
      HAREA = HAREA/SQRT(1.-P0**((1.-GAM)/GAM))
      HAREA = HAREA*P0**(1./GAM)
      HDIA = SQRT(HAREA/A)
      RHOA = RHOE(I)/PE(I)**(1./GAM)
      TA = TE(I)/PE(I)**((GAM-1.)/GAM)
      UA = UE(I)*(A/HAREA)*PE(I)**(1./GAM)
      WRITE(IWRITE,1120) TIME(I),RHOA,TA,UA,XID,SHOCKL,HDIA,
1 CO2(I),CO(I),H2O(I),H2(I)
1120 FORMAT(1P11G10.3)
      70 CONTINUE
C
C ISENTROPIC REGION AND MACH DISC
C
      WRITE(IWRITE,1130)
1130 FORMAT('1',T45,'ISENTROPIC REGION FLOW FIELD'//
1 T5,'TIME',T20,'R/D',T35,'MACH NO.',T50,'RHO',T65,
2 'PRESSURE',T80,'TEMPERATURE',T95,'VELOCITY'/
3 T6,'MSEC',T50,'KG/M3',T66,'ATM',T81,'DEG K',T96,'M/SEC'/)
C
      DO 90 KK=5,JJ,5
      XID = .69*SQRT(GAM*PE(KK))
      XID = XID/(1. + .197*PHI**.65)
      STEP = .1*XID
      ROVERD = .69*SQRT(2.*GAM) - STEP
80 ROVERD = ROVERD + STEP
      IF(ROVERD.GE.XID) ROVERD = XID
      CALL MACHN(ROVERD,FMACH,PHI,GAM,XID)
      RHOI = RHOE(KK)*((1.+GAM)/(2.+(GAM-1.)*FMACH*FMACH))**
1(1./(GAM-1.))
      RATIO = RHOI/RHOE(KK)
      PI = PE(KK)*(RATIO)**GAM
      TI = TE(KK)*(RATIO)**(GAM-1.)
      UI = UE(KK)*FMACH*(RATIO)**(.5*(GAM-1.))
      WRITE(IWRITE,1140) TIME(KK),ROVERD,FMACH,RHOI,PI,TI,UI

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```

1140 FORMAT(1P7G15.4)
      IF(ROVERD.LT.XID) GO TO 80
      FMACHS = FMACH*FMACH
      FMACH2 = (1. + .5*(GAM-1.)*FMACHS)/(GAM*FMACHS-.5*(GAM-1.))
      FMACH2 = SQRT(FMACH2)
      RHOMD2 = RHOI*(GAM+1.)*FMACHS/((GAM-1.)*FMACHS+2.)
      PMD2 = 1.
      TMD2 = TE(KK)*(2.*GAM*FMACHS-GAM+1.)/(GAM+1.)/FMACHS
      UMD2 = RHOI/RHOMD2*UI
      WRITE(IWRITE,1150) TIME(KK),ROVERD,FMACH2,RHOMD2,PMD2,TMD2,UMD2
1150 FORMAT(1P7G15.4//)
      90 CONTINUE

C
      WRITE(IWRITE,1160)
1160 FORMAT('0',' THIS IS THE END OF THE PROGRAM''S OUTPUT')
C
      STOP
      END

C
C
C
      SUBROUTINE ZTHETA(Delta Tau,DLTAU0,THET0,THET0P,IMAX,M,I,
1 G10,EJECTO)
C
C ZTHETA DETERMINES Z(TAU) AND THETA(TAU) USING
C RUNGE-KUTTA INTEGRATION SCHEME
C   IMAX=DIMENSION OF Z IN MAIN PROGRAM
C   I=HIGHEST SUBSCRIPT FOR WHICH VALUES STORED IN Z
C   M=NUMBER OF ITERATIONS BETWEEN STORRED VALUES
      DOUBLE Y(20),DERY(20),Q(20),G1,G1P
      REAL M0,LAMM
C   EXTERNAL DERIV
      COMMON /G/ Q,A(4),B(4),C(4)
      COMMON/WORKB/THETA(500),Z(500),H1(500),H1P(500),THETAP(500),
1 TTAU(500),FEJECT(500)
      COMMON/WORKA/LAMM,GAM,EPS,M0,B0,C0,D0,KPMAX
C
C INITIAL CONDITIONS
C
      THETA(1)=THET0+THET0P*DLTAU0
      TAU=DLTAU0
      TTAU(1) = DLTAU0
      Y(1)=THETA(1)
      DERY(1) = THET0P
      EXPON = -.5*(GAM+1.)
C
C DERIV DETERMINES DY/DX AND THE VALUES OF G1 AND G1P
C
C   CALL DDERIV
      NSUB=1
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
C   CALL DERIV(TAU,Y,DERY,G1,G1P)
      NSUB=2
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
      Z(1)= Y(2)

```

```

      THETAP(1) = DERY(1)
      H1(1)=Y(1)*G1
      H1P(1)=DERY(1)*G1+Y(1)*G1P
      FEJECT(1) = .5*(((THET0*G10-EPS)**EXPON) +((Y(1)*G1-EPS)
1**EXPON))*DLTAU0
      EJECT = FEJECT(1)
      G1OLD = G1
C
C GILL INITIALIZES RUNGE - KUTTA ROUTINE GILL1
C
C      CALL GILL(1,Q,DERIV)
      CALL GILL(1)
      I=1
10 I=I+1
      IF(I.GE.IMAX) GO TO 50
C
C GILL1 INTEGRATES ONE STEP REPLACING TAU AND Y WITH NEW VALUES
C
      Y1OLD = THETA(I-1)
      Y2OLD=Z(I-1)
C
      DO 30 J=1,M
      CALL GILL1(DELTAU,TAU,Y,DERY)
C
C STOPING CONDITION: Z(TAU0)=0 ; LINEAR INTERPOLATION DETERMINES
C TAU0 & THETA(TAU0)
C
      IF(Y(2).GE.0.0) GO TO 20
      R=Y2OLD/Y(2)
      TAU0=TAU-DELTAU/(1.-R)
      TTAU(I) = TAU0
      Y(2) = 0.
      Z(I) = Y(2)
C
      SLOPE = (Y(1)-Y1OLD)/DELTAU
      Y(1) = SLOPE*(TAU0-TAU) + Y(1)
      THETA(I)=Y(1)
C
C      CALL DERIV(TAU0,Y,DERY,G1,G1P)
      NSUB=2
      CALL DERIV(TAU0,Y,DERY,G1,G1P,NSUB)
      THETAP(I) = DERY(1)
      H1(I)=Y(1)*G1
      H1P(I)=DERY(1)*G1+Y(1)*G1P
      FEJECT(I) = EJECT+.5*(((Y1OLD*G1OLD-EPS)**EXPON)+
1((Y(1)*G1-EPS)**EXPON))*DELTAU
      EJECTO = .5*((Y(1)*G1-EPS)**EXPON)*DELTAU
      RETURN
C 20 CALL DERIV(TAU,Y,DERY,G1,G1P)
20 NSUB=2
      CALL DERIV(TAU,Y,DERY,G1,G1P,NSUB)
      EJECT = EJECT +.5*(((Y1OLD*G1OLD-EPS)**EXPON)+
1((Y(1)*G1-EPS)**EXPON))*DELTAU
      G1OLD = G1
      Y1OLD = Y(1)

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      Y2OLD = Y(2)
30 CONTINUE
C
      THETA(I)=Y(1)
      TTAU(I) = TAU
      Z(I) =Y(2)
      THETAP(I) = DERY(1)
      H1(I)=Y(1)*G1
      H1P(I)=DERY(1)*G1+Y(1)*G1P
      FEJECT(I) = EJECT
C
      GO TO 10
C
50 RETURN
      END
      SUBROUTINE DERIV(TAU,Y,DERY,G1,G1P,NSUB)
C      SUBROUTINE DDERIV
C      DERIV CALCULATES DY/DX      Y(1)=THETA      DERY(1)=THETP
C      Y(2)=Z      DERY(2)=ZP
      DOUBLE Y(2),DERY(2),G1,G1P,B,C,F,F1,F2
      REAL M0,LAMM
      COMMON /WORKA/LAMM,GAM,EPS,M0,B0,C0,D0,KPMAX
C
      IF(NSUB.NE.1) GO TO 30
C
C      CONSTANTS
      AA=LAMM/(GAM*M0*M0)
      A1=AA/(2.-GAM)
      A2=1.+EPS-LAMM/(6.*GAM)+AA/(GAM-1.)
      A3=A1/(1.-GAM)
      A4=LAMM/(2.*GAM)
      A8=1.+EPS-AA*.5
      A9=-1.*EPS*(GAM+1.)*.5
      A10=(1.-GAM)*A1*.5
C
      BB = GAM - 1.
      BBB = 2. - GAM
      B1 = 1. + AA/BB - 2./(BB*M0)*(1.+AA/(3.*BB))
      B2 = 2./(BB*M0)
      B3 = 1. - AA/2.
      B4 = -.5*AA*BB/BBB
      B5 = -.5*EPS*BB
      B6 = (GAM + 1. )*AA/(6.*BB*BBB)
      B7 = -1.*AA/BBB
      B8 = AA/(BB*BBB)
C
      RETURN
C
C      CALL DERIV(TAU,Y,DERY,G1,G1P)
30 CONTINUE
C      EQUATIONS
C
      F=1.+TAU
C
      F1 = B3 + (B4+B5*TAU)/F + B6/F**BB

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```

F2 = 1. + B7/F + B8/F**BB
Y(2) = F * (B1 + B2/F**(.5*BB) * F1)/F2
C
B=1./F-A1/(F*F)+A1/F**GAM
C=F**(.5*(1.-GAM))*(A8+A9*TAU/F+A10/F+A1*.5/F**(GAM-1.))
DERY(2)=B*Y(2)-C/M0
C
G1=A1+A2*F+A3*F**(2.-GAM)+A4*Y(2)*Y(2)/F
G1P=A2+(2.-GAM)*A3*F**(1.-GAM)+A4*(-1.*Y(2)*Y(2)/(F*F)+
12.*Y(2)*DERY(2)/F)
IF(TAU.EQ.0.) GO TO 60
FACT=Y(1)*G1-EPS
C
WRITE(6,*)FACT
IF(FACT.LT.0.)FACT=1.E-50
DERY(1)=-1.*Y(1)*(1.+Y(1))*G1P/G1+Y(1)/(1.-Y(2))*(C*(1.-Y(1))/M0
1-B*Y(2)*(1.+Y(1))+2.*Y(1)*G1*FACT**(-.5*(GAM+1.))/M0)
C
C
60 CONTINUE
RETURN
END
SUBROUTINE GILL(N)
C
SUBROUTINE GILL(N,Q,DERIV)
C
DOUBLE Y(N),DERY(N),Q(N),G1,G1P,XK,DY
DOUBLE Y(20),DERY(20),Q(20),G1,G1P,XK,DY
COMMON /G/ Q,A(4),B(4),C(4)
DATA A(1),B(1),C(1),C(4)/0.5,-1.0,-0.5,-0.5/
DO 10 I=1,N
10 Q(I)=0.0
C1=1.0/SQRT(2.0)
A(2)=1.0-C1
A(3)=1.0+C1
A(4)=1.0/6.0
B(2)=-A(2)
B(3)=-A(3)
B(4)=-1.0/3.0
C(2)=B(2)
C(3)=B(3)
RETURN
END
SUBROUTINE GILL1(DX,X,Y,DERY)
C
CALL GILL1(DX,X,Y,DERY)
DOUBLE Y(20),DERY(20),Q(20),G1,G1P,XK,DY
COMMON /G/ Q,A(4),B(4),C(4)
DO 30 I=1,4
IF(I.EQ.2.OR.I.EQ.4) X=X+0.5*DX
C
CALL DERIV (X,Y,DERY,G1,G1P)
NSUB=2
CALL DERIV(X,Y,DERY,G1,G1P,NSUB)
DO 30 J=1,N
XK=DX*DERY(J)
DY=A(I)*XK+B(I)*Q(J)
Y(J)=Y(J)+DY
Q(J)=Q(J)+3.0*DY+C(I)*XK
30 CONTINUE

```

```

RETURN
END
SUBROUTINE RATEAU(TSTAR,T20,EJECTO,II,J)
REAL M0,LAMM,L,MP,MACHNO
COMMON/WORKA/LAMM,GAM,EPS,M0,B0,C0,D0,KPMAX
COMMON/WORKB/THETA(500),Z(500),H1(500),H1P(500),THETAP(500),
1 TTAU(500),FEJECT(500)
COMMON/WORKC/TEFF,ETA,A,L,MP,V0,ALMP,R
COMMON/WORKD/PE(50),UE(50),TE(50),RHOE(50),TIME(50),
1 TEMP(50),FKP(50),CO2(50),CO(50),H2O(50),H2(50)
DATA DELTAT/1.E-03/
DATA IWRITE/6/
TSTAR = TSTAR/1000.
THET = (.5*(GAM+1.))**((GAM+1.)/(GAM-1.))/GAM
THET = THET/R/TEFF/(1.+LAMM/6.)/(1.-ETA*LAMM)**(GAM-1.)
THET = 2.*L*(1.+0.13*ETA/ALMP)/(GAM-1.)*SQRT(THET)
T0 = ((1.+LAMM/6.)*TEFF/T20)**(1./(GAM-1.))
T0 = T0*(ALMP-ETA)/(ALMP+1.07*ETA)
T0 = T0 + 2.07*ETA/(ALMP+1.07*ETA)
T0 = THET*(T0**(.5*(GAM-1.)) - 1.)
T = TSTAR - DELTAT
EJECT = FEJECT(II)
J = 0
10 J = J + 1
T = T + DELTAT
TMSEC = 1000.*T
TREPLC = T - TSTAR + T0
RHO2 = (1. + TREPLC/THET)**(2./(GAM-1.))
RHO2 = (ALMP + 1.07*ETA)*RHO2 - 1.07*ETA
RHO2 = 1./RHO2
P2 = R*TEFF*(1.+LAMM/6.)
P2 = P2*(ALMP-ETA)**(GAM-1.)
P2 = P2/(1./RHO2-ETA)**GAM
T2 = P2*(1./RHO2-ETA)/R
V2 = (ALMP-ETA)/(1./RHO2-ETA)
V2 = V0/M0/(1.-ETA*RHO2)*V2**(.5*(GAM-1.))
SONICV = SQRT(GAM*R*T2)
MACHNO = V2/SONICV
P2ATM = P2/101330.
PE(J) = P2ATM
UE(J) = V2
TE(J) = T2
RHOE(J) = RHO2
TIME(J) = TMSEC
C
C DETERMINE THE REACTION RATE CONSTANT FKP
C
TA = T2/P2ATM**((GAM-1.)/GAM)
DO 20 I=1,KPMAX
IF(TA.GE.TEMP(I)) GO TO 20
IF(I.LE.1) GO TO 30
SLOPE = (FKP(I) - FKP(I-1))/(TEMP(I) - TEMP(I-1))
FKPP = SLOPE*(TA - TEMP(I)) + FKP(I)
GO TO 40
20 CONTINUE

```

```

30 WRITE(IWRITE,1000) TMSEC,TA
1000 FORMAT(' EXIT PLANE TEMPERATURE T2 IS OUTSIDE THE RATE',
1 ' CONSTANT INTERPOLATION TABLE RANGE'/' COMPUTATION',
2 ' TERMINATED WITH TIME =',F10.3,' ,T2 =',F10.3/)
40 CONTINUE
C
AA = (D0*FKPP + B0 + C0)**2 + 4.*B0*C0*(FKPP-1.)
AA = SQRT(AA) - D0*FKPP - B0 - C0
AA = AA/(2.*(FKPP-1.))
CO2(J) = AA
CO(J) = B0 - AA
H2O(J) = C0 - AA
H2(J) = D0 + AA
C
IF(J.EQ.1) GO TO 50
EJECTN = .5*A/MP*RHO2*V2*DELTAT
EJECT = EJECT + EJECTN + EJECTO
EJECTO = EJECTN
50 WRITE(IWRITE,1010) TMSEC,RHO2,V2,P2,P2ATM,T2,SONICV,MACHNO,EJECT
1010 FORMAT(' ',1P9G13.4)
IF(P2ATM.LE.1.) RETURN
GO TO 10
END
C
SUBROUTINE MACHN(R,FM,PHI,GAM,XI)
C
C MACHN CALCULATES THE MACH NUMBER GIVEN THE AXIAL DIATANCE
C FROM THE MUZZLE BY HALF INTERVAL SEARCH
C
DATA IWRITE/6/
DATA EPS/.01/
F(X) = SQRT(.49*GAM*(2.+(GAM-1.)*X*X)**(GAM/(GAM-1.)))/
1 (1. + .197*PHI**.65)**2/(2.*GAM*X*X - GAM + 1.)/
2 (GAM+1.)*(1./(GAM-1.)))
FMIN = 1.
FMAX = 1.
DO 10 I=1,20
FMAX = FMAX + FMAX*FMAX
IF(F(FMAX).GE.XI) GO TO 30
10 CONTINUE
DO 20 I=1,200
FM = .5*(FMIN + FMAX)
DELTA = F(FM) - R
IF(ABS(DELTA).LE.EPS) RETURN
IF(DELTA.LE.0.) FMIN = FM
IF(DELTA.GT.0.) FMAX = FM
20 CONTINUE
30 CONTINUE
WRITE(IWRITE,1000) FMIN,FMAX,FM,R,DELTA
1000 FORMAT('WARNING-SUBROUTINE MACHN'S CALCULATION',
1 ' OF MACH NUMBER HAS NOT CONVERGED AFTER 200 ITERATIONS'/
2 ' FMIN =',1PG10.3,' FMAX =',G10.3,' FM =',G10.3,' R =',
3 G10.3,' DELTA =',G10.3)
STOP
END

```

APPENDIX F  
MTOB PROGRAM LISTING

```

      PROGRAM MTOB(INPUT,OUTPUT,TAPE9,TAPE4,TAPE8,TAPE6=OUTPUT)
C
C TAPE8 IS OUTPUT TAPE FOR BLAKE, CONCEN, AND LAPP
C TAPE9 IS INPUT TAPE FROM MEFF
C TAPE4 IS INPUT BOILERPLATE FOR THE APPROPRIATE GAS
C
      DIMENSION A(30,80),TITLE(20)
      REWIND 4
      REWIND 8
      REWIND 9
C
C READ THE RESULTS OF THE MEFF CALCULATION
      READ(9,400)TITLE
      READ(9,300)T1,T2,T3,P,V,ALPHA,RADIUS,XMAX,PRNT,FDL,KEY
C
C NOW READ THE BLAKE BOILERPLATE
      DO 20 I=1,30
      IF(EOF(4))30,20
      20 READ(4,100)(A(I,J),J=1,80)
C
C HERE ONCE BOILERPLATE FILE IS READ
      30 II=I-2
C
      DO 40 K=1,II
      40 WRITE(8,100)(A(K,J),J=1,80)
C
C NOW FOR THE SPECIAL LINES
C
      50 WRITE(8,120)
      120 FORMAT(9HPRL,CON,2)
      WRITE(8,110)T1
      110 FORMAT(11HPOI,P,1.,T,,F8.3)
      WRITE(8,130)P,T2
      130 FORMAT(6HPOI,P,,F8.3,3H,T,,F8.3)
      WRITE(8,170)
      170 FORMAT(4HQUIT)
      WRITE(8,180)ALPHA
      180 FORMAT(F8.3)
      WRITE(8,400) TITLE
      WRITE(8,190)RADIUS,XMAX,PRNT
      190 FORMAT(3E10.3)
      WRITE(8,210)FDL,KEY
      210 FORMAT(F8.3,I1)
      WRITE(8,200)T3,V
      200 FORMAT(2F8.3,/,4H*EOI)
      300 FORMAT(10F8.3,I1)
      100 FORMAT(80A1)
      400 FORMAT(20A4)
      END

```

APPENDIX G  
BOIL LISTING

TIT, M30A1  
PRL, CON, 2  
REJ, N, K2SO4, C, C2, CH, CH2O, HNO3  
REJ, C(S), K2SO4\$  
REJ, KOH\$, KO2\$, K2O2\$  
REJ, H2S, S2O, SO2, K\$, K2O, K2O2  
REJ, KCO\$, KSO\$, K2O\$, K\$  
REJ, K2CO3\$  
REJ, K2S\$  
UNI, ENG  
CM2, NC1260, 27.9, NG, 22.42, NQ, 46.84, EC, 1.49, KS, 1.,  
ALC, .25, C, .1

APPENDIX H  
CONCEN PROGRAM LISTING

```

      PROGRAM CONCEN(INPUT,OUTPUT,TAPE1,TAPE2,TAPE5=INPUT,
+ TAPE6=OUTPUT,TAPE8)
C
C 13 SPECIES
C
      DIMENSION NAM(17),CONC(17,2),NA(2,29),CO(2,29)
      DIMENSION CON(17),SUM(2)
      DATA CONST/'CONST'/
C
C THE NAME OF EACH SPECIES MUST BE 4 CHARACTERS
C
      DATA NAM/' H2O',' CO',' H2',' N2',' CO2',' H',' OH',' O',
+ ' O2',' K',' KOH',' KO2',' HO2'/
      REWIND 1
      REWIND 2
      READ(8,300)ALPHA
      NSPEC=13
      K=0
      I=0
      SUM(1)=0.
      SUM(2)=0.
1 READ(1,200)ALINE
  IF(ALINE.NE.CONST)GOTO 1
  I=I+1
  READ(1,200)JUNK
  DO 10 J=1,29
    READ(1,100)NA(I,J),CO(I,J)
    IF(NA(I,J).EQ.' ')GOTO 20
10 CONTINUE
20 IF(I.EQ.1)GOTO 1
50 K=K+1
  DO 30 I=1,NSPEC
    DO 40 J=1,29
      IF(NA(K,J).EQ.NAM(I))CONC(I,K)=CO(K,J)
40 CONTINUE
30 CONTINUE
  DO 60 L=1,NSPEC
60 CONTINUE
    IF(K.EQ.1)GOTO 50
    DO 70 I=1,2
      DO 80 J=1,NSPEC
        SUM(I)=SUM(I)+CO(I,J)
80 CONTINUE
70 CONTINUE
      WRITE(6,400)
      WRITE(6,500)ALPHA
      DO 90 I=1,NSPEC
        CON(I)=(1.-ALPHA)*(CONC(I,1)/SUM(1))+ALPHA*(CONC(I,2)/SUM(2))
        WRITE(6,400)NAM(I),CON(I)
90 CONTINUE
      WRITE(2,700)(CON(I),I=1,NSPEC)
      WRITE(6,600)
      STOP
100 FORMAT(4X,A4,14X,1PE11.5)
200 FORMAT(9X,A5)

```

```
300 FORMAT(F8.3)
400 FORMAT(2X,A4,5X,1PE10.3)
500 FORMAT(1H1,2X,' ALPHA= ',F5.3)
600 FORMAT(1H1)
700 FORMAT(7E10.4)
END
```

APPENDIX I  
LASTDA DATA LISTING

	13	13	6	42	0	0	0	200	0	22		
	0.	99.99		9.99			1.		1.	999.999		1.
	.1E-10	.999										
	1.00	999.9		294.			9999.		0.1			200.
	.1E-50	.1E-50		.1E-50			.79		.00032	.1E-50		.1E-50
	.1E-50	.21		.1E-50			.1E-50		.1E-50	.1E-50		
H2O	18.016	-57.7979										
	100.	7.961		52.202			-1.581		200.	7.969		45.837
	400.	8.186		45.422			0.825		600.	8.676		46.710
	800.	9.246		48.089			4.300		1000.	9.851		49.382
	1200.	10.444		50.575			8.240		1400.	10.987		51.675
	1600.	11.462		52.698			12.630		1800.	11.869		53.652
	2000.	12.214		54.548			17.373		2200.	12.505		55.392
	2400.	12.753		56.190			22.372		2600.	12.965		56.947
	2800.	13.146		57.667			27.556		3000.	13.304		58.354
	3200.	13.441		59.010			32.876		3400.	13.562		59.639
	3600.	13.669		60.242			38.300		3800.	13.764		60.821
	4000.	13.850		61.379			43.805		4200.	13.927		61.917
CO	28.01055	-26.42										
	100.	6.956		53.401			-1.379		200.	6.957		47.851
	400.	7.013		47.488			0.711		600.	7.276		48.591
	800.	7.624		49.759			3.627		1000.	7.931		50.845
	1200.	8.168		51.834			6.794		1400.	8.346		52.736
	1600.	8.480		53.562			10.130		1800.	8.583		54.322
	2000.	8.664		55.026			13.561		2200.	8.728		55.680
	2400.	8.781		56.292			17.052		2600.	8.825		56.866
	2800.	8.863		57.407			20.582		3000.	8.895		57.917
	3200.	8.924		58.401			24.139		3400.	8.949		58.861
	3600.	8.973		59.299			27.719		3800.	8.994		59.717
	4000.	9.014		60.117			31.316		4200.	9.033		60.501
H2	2.016	0.0										
	100.	5.393		37.035			-1.265		200.	6.518		31.831
	400.	6.975		31.480			0.707		600.	7.009		32.573
	800.	7.087		33.715			3.514		1000.	7.219		34.758
	1200.	7.390		35.696			6.404		1400.	7.600		36.543
	1600.	7.823		37.314			9.446		1800.	8.016		38.022
	2000.	8.195		38.678			12.651		2200.	8.358		39.290
	2400.	8.506		39.863			15.993		2600.	8.639		40.402
	2800.	8.757		40.912			19.448		3000.	8.859		41.395
	3200.	8.962		41.855			22.992		3400.	9.061		42.294
	3600.	9.158		42.714			26.616		3800.	9.252		43.116
	4000.	9.342		43.502			30.317		4200.	9.429		43.874
N2	28.0134	0.0										
	100.	6.956		51.957			-1.379		200.	6.957		46.407
	400.	6.990		46.043			0.710		600.	7.196		47.143
	800.	7.512		48.303			3.596		1000.	7.815		49.378
	1200.	8.061		50.357			6.718		1400.	8.252		51.248
	1600.	8.398		52.065			10.015		1800.	8.512		52.816
	2000.	8.601		53.513			13.418		2200.	8.672		54.160
	2400.	8.731		54.766			16.886		2600.	8.779		55.335
	2800.	8.820		55.870			20.398		3000.	8.855		56.376
	3200.	8.886		56.856			23.939		3400.	8.914		57.312
	3600.	8.939		57.747			27.505		3800.	8.962		58.162
	4000.	8.983		58.559			31.089		4200.	9.002		58.940

CO2	44.053	-94.054					
100.	6.981	58.188	-1.543	200.	7.734	51.849	-0.816
400.	9.877	51.434	0.958	600.	11.310	52.981	3.087
800.	12.293	54.706	5.453	1000.	12.980	56.359	7.984
1200.	13.466	57.896	10.632	1400.	13.815	59.315	13.362
1600.	14.074	60.627	16.152	1800.	14.269	61.843	18.987
2000.	14.424	62.974	21.857	2200.	14.547	64.031	24.755
2400.	14.643	65.023	27.674	2600.	14.734	65.956	30.613
2800.	14.807	66.836	33.567	3000.	14.873	67.670	36.535
3200.	14.930	68.461	39.515	3400.	14.982	69.215	42.507
3600.	15.030	69.933	45.508	3800.	15.075	70.620	48.518
4000.	15.119	71.278	51.538	4200.	15.159	71.909	54.566
H	1.00797E0	52.1					
100.	4.968	31.809	-0.984	200.	4.968	27.847	-0.488
400.	4.968	27.587	0.506	600.	4.968	28.367	1.500
800.	4.968	29.179	2.493	1000.	4.968	29.917	3.487
1200.	4.968	30.576	4.481	1400.	4.968	31.166	5.474
1600.	4.968	31.697	6.468	1800.	4.968	32.179	7.461
2000.	4.968	32.621	8.455	2200.	4.968	33.027	9.449
2400.	4.968	33.403	10.442	2600.	4.968	33.753	11.436
2800.	4.968	34.081	12.430	3000.	4.968	34.388	13.423
3200.	4.968	34.678	14.417	3400.	4.968	34.952	15.410
3600.	4.968	35.212	16.404	3800.	4.968	35.459	17.398
4000.	4.968	35.694	18.391	4200.	4.968	35.919	19.385
OH	17.0074	9.492					
100.	7.798	50.398	-1.467	200.	7.356	44.541	-0.711
400.	7.087	44.160	0.725	600.	7.057	45.275	2.137
800.	7.150	46.432	3.556	1000.	7.332	47.488	5.003
1200.	7.549	48.437	6.491	1400.	7.766	49.296	8.023
1600.	7.963	50.079	9.596	1800.	8.137	50.799	11.207
2000.	8.286	51.466	12.849	2200.	8.415	52.087	14.520
2400.	8.526	52.668	16.214	2600.	8.622	53.214	17.929
2800.	8.706	53.730	19.622	3000.	8.780	54.218	21.411
3200.	8.846	54.682	23.174	3400.	8.905	55.124	24.949
3600.	8.959	55.546	26.735	3800.	9.009	55.950	28.532
4000.	9.054	56.337	30.339	4200.	9.097	56.709	32.154
O	16.000	59.559					
100.	5.666	43.266	-1.080	200.	5.434	38.953	-0.523
400.	5.135	38.672	0.528	600.	5.049	39.480	1.544
800.	5.015	40.313	2.550	1000.	4.999	41.067	3.552
1200.	4.990	41.737	4.551	1400.	4.984	42.335	5.548
1600.	4.981	42.873	6.544	1800.	4.979	43.361	7.540
2000.	4.978	43.806	8.536	2200.	4.979	44.216	9.532
2400.	4.981	44.596	10.527	2600.	4.986	44.948	11.524
2800.	4.994	45.278	12.522	3000.	5.004	45.588	13.522
3200.	5.017	45.880	14.524	3400.	5.033	46.156	15.529
3600.	5.050	46.418	16.537	3800.	5.070	46.667	17.549
4000.	5.091	46.904	18.565	4200.	5.114	47.131	19.586
O2	31.9988	0.0					
100.	6.958	55.205	-1.381	200.	6.961	49.643	-0.685
400.	7.196	49.282	0.724	600.	7.670	50.414	2.210
800.	8.063	51.629	3.786	1000.	8.336	52.765	5.427
1200.	8.527	53.801	7.114	1400.	8.674	54.744	8.835
1600.	8.800	55.608	10.583	1800.	8.916	56.401	12.354
2000.	9.029	57.136	14.149	2200.	9.139	57.819	15.966

	2400.	9.248	58.457	17.804	2600.	9.354	59.057	19.664
	2800.	9.455	59.622	21.545	3000.	9.551	60.157	23.446
	3200.	9.640	60.665	25.365	3400.	9.723	61.149	27.302
	3600.	9.799	61.611	29.254	3800.	9.869	62.053	31.221
	4000.	9.932	62.476	33.201	4200.	9.988	62.883	35.193
K	39.100	21.31						
	100.	4.968	42.714	-.984	200.	4.968	38.751	-.488
	400.	4.968	38.492	.506	600.	4.968	39.272	1.500
	800.	4.968	40.084	2.493	1000.	4.968	40.822	3.487
	1200.	4.968	41.481	4.481	1400.	4.970	42.070	5.474
	1600.	4.975	42.602	6.469	1800.	4.988	43.084	7.465
	2000.	5.013	43.526	8.465	2200.	5.057	43.932	9.471
	2400.	5.122	44.310	10.489	2600.	5.213	44.662	11.522
	2800.	5.334	44.993	12.576	3000.	5.489	45.305	13.658
	3200.	5.685	45.601	14.775	3400.	5.932	45.883	15.935
	3600.	6.242	46.153	17.152	3800.	6.630	46.412	18.438
	4000.	7.111	46.664	19.810	4200.	7.701	46.908	21.289
KOH	56.109	-55.6						
	100.	7.874	65.898	-2.017	200.	10.439	57.500	-1.090
	400.	12.136	56.932	1.212	600.	12.578	58.830	3.690
	800.	12.835	60.845	6.232	1000.	13.083	62.702	8.824
	1200.	13.327	64.379	11.465	1400.	13.551	65.895	14.154
	1600.	13.746	67.275	16.884	1800.	13.911	68.539	19.650
	2000.	14.048	69.706	22.446	2200.	14.162	70.788	25.268
	2400.	14.257	71.798	28.110	2600.	14.336	72.743	30.970
	2800.	14.403	73.632	33.844	3000.	14.459	74.472	36.730
	3200.	14.506	75.266	39.626	3400.	14.547	76.021	42.532
	3600.	14.582	76.739	45.445	3800.	14.612	77.425	48.364
	4000.	14.638	78.080	51.289	4200.	14.661	78.708	54.219
KO2	71.1	-15.0						
	100.	9.925	75.72	-2.133	200.	10.810	67.02	-1.095
	400.	12.086	66.45	1.205	600.	12.830	68.35	3.704
	800.	13.216	70.38	6.313	1000.	13.438	72.26	8.979
	1200.	13.587	73.97	11.682	1400.	13.687	75.52	14.411
	1600.	13.749	76.92	17.155	1800.	13.784	78.20	19.908
	2000.	13.799	79.38	22.667	2200.	13.803	80.47	25.427
	2400.	13.801	81.49	28.188	2600.	13.797	82.43	30.948
	2800.	13.797	83.32	33.707	3000.	13.802	84.16	36.467
	3200.	13.814	84.94	39.228	3400.	13.831	85.69	41.993
	3600.	13.855	86.40	44.761	3800.	13.881	87.07	47.535
	4000.	13.905	87.72	50.313	4200.	13.925	88.33	53.097
HO2	33.008	0.5						
	100.	7.949	61.574	-1.596	200.	8.003	55.132	-0.799
	400.	8.907	54.717	0.877	600.	9.980	56.116	2.771
	800.	10.769	57.657	4.850	1000.	11.365	59.123	7.066
	1200.	11.831	60.481	9.387	1400.	12.197	61.734	11.791
	1600.	12.485	62.891	14.261	1800.	12.714	63.965	16.782
	2000.	12.895	64.966	19.343	2200.	13.041	65.902	21.937
	2400.	13.160	66.781	24.558	2600.	13.256	67.610	27.200
	2800.	13.336	68.393	29.859	3000.	13.403	69.135	32.534
	3200.	13.459	69.840	35.220	3400.	13.507	70.511	37.917
	3600.	13.547	71.153	40.622	3800.	13.582	71.766	43.335
	4000.	13.612	72.354	46.055	4200.	13.638	72.918	48.780
CO	+0	+M	=CO2	+M	26	7.0E-33	0.	-4369.
CO	+02	+	=CO2	+0	15	4.2E-12	0.	-47664.

O	+O	+M	=O2	+M	25	3.0E-34	0.	1792.0
CO	+OH	+	=CO2	+H	16	2.8E-17	-1.3	660.0
OH	+H2	+	=H2O	+H	161.90E-15	-1.3		-3626.
H	+O2	+	=OH	+O	152.40E-10	0.		-16393.
O	+H2	+	=OH	+H	16	3.0E-14	-1.	-8902.
OH	+OH	+	=H2O	+O	151.05E-11	0.		-1093.
H	+H	+M	=H2	+M	223.00E-30	1.		0.
H	+OH	+M	=H2O	+M	231.00E-25	2.		0.
H	+O2	+M	=H02	+M	25	1.5E-32	0.	994.
H	+H02	+	=OH	+OH	15	1.7E-10	0.	-994.
CO	+H02	+	=CO2	+OH	15	2.5E-10	0.	-23645.
H	+H02	+	=H2	+O2	15	4.2E-11	0.	-695.
H	+H02	+	=H2O	+O	15	8.5E-12	0.	-994.
OH	+H02	+	=H2O	+O2	11	3.0E-11	0.	0.
O	+H02	+	=OH	+O2	11	3.5E-11	0.	0.
O	+H	+M	=OH	+M	22	1.0E-29	1.	0.
H02	+H2	+	=H2O	+OH	15	1.0E-12	0.	-18678.
H	+KOH	+	=H2O	+K	15	1.8E-11	0.	-1987.
K	+OH	+M	=KOH	+M	22	1.5E-27	1.	0.
K02	+OH	+	=KOH	+O2	11	2.0E-11	0.	0.
K	+O2	+M	=K02	+M	22	3.0E-30	1.	0.
K	+H02	+	=K02	+H	15	1.0E-11	0.	-13000.
K02	+H2	+	=KOH	+OH	15	3.0E-12	0.	-19870.

APPENDIX J  
LAPP PROGRAM LISTING

```

C
C RELEASE VERSION OF LAPP MODIFIED TO ACCEPT UP THROUGH 49 REACTIONS.
C   MARCH 1983
C
C
C   PROGRAM LAPP(INPUT,OUTPUT,TAPE2,TAPE3,TAPE5=INPUT,TAPE6=OUTPUT,
+   TAPE7,TAPE8,TAPE10,TAPE11,TAPE12)
C
C TAPE2 IS INPUT FROM PROGRAM CONCEN
C TAPE3 IS INPUT FROM FILE OF LAPP DATA
C TAPE8 IS INPUT FROM PROGRAM MTOB
C
C*****
C*****
C*****      AXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY      **
C*****      AEROCHEM RESEARCH LABORATORIES                          **
C*****      PRINCETON, N. J.                                         **
C*****
C*****
C   DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
2   WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),
3RU(30),U(30),TITLE(12),XLE(30),XMU(30),G(25),WTMIX(30),
4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),
5   IRR(49),FREQ(30),SAVEA(25,30),PC(4),ZID(5),
6   ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),
7T4(30),TFDG(30),IRT(49),RP(49,30),RM(49,30)
C   DIMENSION XAME(6), ISAVE(6), FREQA(6), ALOC(50,6)
C   DIMENSION TTB(30,24),CPTB(25,30),HTB(25,30),GTB(25,30),HF(25)
C   DIMENSION TABLE(16),ZSPEC(16)
C   COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
C   COMMON/UNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,
*NUNITG,NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NUNITN,
*NOUT,NDBG,NNNOUT
C   COMMON/A/ CM(25,25,26),CM1(25,25),QX(25,26),QX1(25)
C   COMMON/C/ IZSPEC,ISPEC(16)
C   COMMON  A      , RHO      , Y      , T      , PSI      , RT
C   COMMON  SUM    , AR      , HSTAT  , H      , ALPHA    , RALPHA
C   COMMON  CP     , SIGMA   ,        ,        , WTMOLE   , CPBAR   , C
C   COMMON  AID    , ETA     , RATIO   , RU     , U      , TITLE
C   COMMON  XLE    , XMU     ,        , G      , WTMIX   , WDOT
C   COMMON  SAVEU  , SAVET   , WM     , WP     , RC
C   COMMON        , SAVEA   ,        , PC     , X      , XMAX
C   COMMON  PRNT   , DXMIN   , DX     , FDL    , DELPSI  , RJ
C   COMMON  XK2    , P      , ZID    , FREQ   , ECC     , DPDX
C   COMMON  YOUT   , HOUT    , RHOOUT , IRRR   , IRR     , IFINIS
C   COMMON  IPAGE  , MPSI    , MY     , NS     , NR      , IEDGE
C   COMMON  ITURB  , IPRESS  , NPSI   , ITEST  , ITER    , IECC
C   COMMON  IRT    , XMUOUT  , XLT    , T4     , TFDG    , IOUT
C   COMMON  IOUT1  , IOUT2   , RP     , RM     , ISAVE   , IPUNCH
C   COMMON TKINET,NFREQA,ALOC,FREQA,QQ100,QQ200,QQ300,QQ400
C
C**** SETTING XAME FOR THOSE SPECIES INVOLVED IN COLLISION FREQ. CALC.
C
C   DATA XAME(1)/6HCO /

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DATA XAME(2)/6HCO2 /
DATA XAME(3)/6HH2O /
DATA XAME(4)/6HH2 /
DATA XAME(5)/6HN2 /
DATA XAME(6)/6HHCL /
DATA TABLE/8HCO ,8HHCL ,8HH2O ,8HOH ,
1      8HCO2 ,8HHF ,8HCN ,8HO ,
2      8HBF ,8HBFO ,8HBHO2 ,8HBF2 ,
3      8HBF3 ,8HBO ,8H ,8HAL2O3 /
C
CCCCC COMMENT OUT NAMELIST DEFINITION WHICH FOLLOWS IF PROCESS NAMELIST
CCCCC BY CALLS TO SUBROUTINE NMLST....ALSO COMMENT OUT NORMAL READS
CCCCC AND WRITES FOR IBM SUPPORTED NAMELIST
CCCCC NAMELIST/NUNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,NUNITG,
CCCCC*NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NOUT,NDBG
C
C      INITIALIZE VARIABLES
      AMULT=0.3048
      AMULT3=14.5939
      JPROC=2
      NUNITA=2
      NUNITB=3
      NUNITC=5
      NUNITD=7
      NUNITE=7
      NUNITF=8
      NUNITG=0
      NUNITH=0
      NUNITI=0
      NUNITJ=0
      NUNITK=0
      NUNITL=0
      NUNITM=0
      NUNITN=5
      NOUT=6
      NINOUT=6
      NNNOUT=10
      NDBG=6
C
      AV=6.025E23
C... SET CONVERSION TO ENGLISH UNITS MULTIPLIERS
      AMULT1=AMULT*AMULT
      AMULT2=AMULT*AMULT1
      AMULT3=SQRT(AMULT3)
4 IFINIS=0
DO 9999 I=1,8536
9999 A(I)=0.0
DO 300 I = 1,6
300 ISAVE(I) = 0
R=82.06
C..... BEGIN TO INPUT FILE DESIGNATED BY NUNITB
      READ (NUNITF,333)(TITLE(I),I=1,10)
      IF(NUNITM.LT.0)WRITE(NNOUT,333) (TITLE(I),I=1,10)
C
C      NS= NO. OF SPECIES

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C      NR= NO. OF REACTIONS
C
C
      READ(NUNITB,100) MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,
      *IPRESS,NT
      IF(NUNITM.LT.0)WRITE(NNOUT,100) MPSI,NS,ITURB,NR,IOUT1,IOUT2,
      *IPUNCH,ITIME,IPRESS,NT
      READ (NUNITB,111) (FREQA(I), I=1,6)
      IF(NUNITM.LT.0) WRITE(NNOUT,111) (FREQA(I),I=1,6)
      DO 113 I=1,6
      IF (FREQA(I)) 113, 114, 113
113 CONTINUE
      I=7
114 NFREQA = I-1
      NPSI=MPSI-1
      READ (NUNITB,1000)X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2
      READ(NUNITF,1000)RJ,XMAX,PRNT
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK
      X=X/AMULT
      XMAX=XMAX/AMULT
      PRNT=PRNT/AMULT
      RJ=RJ/AMULT
      DX=0.1*RJ
C
C      INPUT MINIMUM STEPSIZE LIMIT (DXMIN)
C
      READ(NUNITB,555) DXMIN,FDL,PC(1),PC(2),PC(3),PC(4),THOT,TCOOL
      READ(NUNITF,556)FDL,KEY
556 FORMAT(F8.3,I1)
      IF(NUNITM.LT.0) WRITE(NNOUT,555)DXMIN,FDL,(PC(KI),KI=1,4),THOT,
      *TCOOL
      IF(KEY.EQ.1)GOTO 98765
      NOUT=10
      NNOUT=10
      NCBG=10
      NNNOUT=6
98765 DXMIN=DXMIN/AMULT
      PC(2)=PC(2)*AMULT
      PC(3)=PC(3)*AMULT1
      PC(4)=PC(4)*AMULT2
      READ (NUNITB,1000)P,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET
      READ(NUNITF,987)T(1),U(1)
987 FORMAT(2F8.3)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)P,T(1),T(MPSI),U(1),U(MPSI),
      *DELPSI,TKINET
      U(1)=U(1)/AMULT
      U(MPSI)=U(MPSI)/AMULT
      DELPSI=DELPSI/AMULT3
      IF(TKINET.EQ.0.0) TKINET = 400.0
C
C**** THE VALUE OF 30 SECONDS IS TO ALLOW FOR COMPILE TIME
C
      ILIMIT = 60*ITIME
      IDIFFT = 0
      CALL TICK(ISECST)

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      IF((ISECST+60*ITIME).GT.86400) IDIFFT = 86400-ISECST
      UNIT = U(1)
      IQ77 = 2
      USUB01 = 0.0
C
C   TURBULENCE MODELS
C
      IF (ITURB - 3) 8600,9010,9010
8600 IF (ITURB - 1) 9011,9010,9011
9010 USUB01 = 0.95* (U(1)-U(MPSI)) + U(MPSI)
9011 CONTINUE
      IF(DELPsi) 3011,3012,3011
C
C**** READING OF CENTERLINE CONCENTRATIONS FROM FILE PRODUCED
C**** BY BLAKE AND CONCEN.
C
3012 READ (NUNITA,1000)(ALPHA(J,1),J=1,NS)
C
C BE SURE NO DENSITIES ARE ZERO
      DO 7777 IJK=1,NS
      ALPHA(IJK,1)=AMAX1(ALPHA(IJK,1),1.E-99)
7777 CONTINUE
C
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)(ALPHA(J,1),J=1,NS)
C
C**** NOW READ THE CONCENTRATIONS ON THE EDGES - AMBIENT AIR.
C
      READ(NUNITB,1000)(ALPHA(J,MPSI),J=1,NS)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)(ALPHA(J,MPSI),J=1,NS)
      MMOD=MPSI-2
      DO 4001 I=1,MMOD
      T(I)=T(1)
      U(I)=U(1)
      DO 4001 J=1,NS
4001 ALPHA(J,I)=ALPHA(J,1)
      DO 4002 J=1,NS
4002 ALPHA(J,NPSI)=ALPHA(J,MPSI)
      GO TO 3015
3011 READ (NUNITB,1000)(T(I),I=1,MPSI)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)(T(I),I=1,MPSI)
      READ (NUNITB,1000)(U(I),I=1,MPSI)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)(U(I),I=1,MPSI)
      DO 7 I=1,MPSI
      U(I)=U(I)/AMULT
      READ (NUNITB,1000)(ALPHA(J,I),J=1,NS)
      IF(NUNITM.LT.0) WRITE(NNOUT,1000)(ALPHA(J,I),J=1,NS)
      7 CONTINUE
C
C   NEW THERMO DATA DATA INPUT IN JANNAF TABLE FORM
C
3015 DO 1991 I=1,NS
      READ(NUNITB,222) AID(I),WTMOLE(I),HF(I)
      IF(NUNITM.LT.0) WRITE(NNOUT,222) AID(I),WTMOLE(I),HF(I)
      DO 10 IT=1, NT,2
      ITP1=IT+1

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      READ(NUNITB,102) TTB(IT,I), CPTB(I,IT),GTB(I,IT),HTB(I,IT),
      *TTB(ITP1,I),CPTB(I,ITP1),GTB(I,ITP1),HTB(I,ITP1)
      IF(NUNITM.LT.0) WRITE(NNOUT,102)TTB(IT,I),CPTB(I,IT),GTB(I,IT),
      *HTB(I,IT),TTB(ITP1,I),CPTB(I,ITP1),GTB(I,ITP1),HTB(I,ITP1)
      GTB(I,IT)= -GTB(I,IT)*TTB(IT,I) +HF(I) *1000.
      GTB(I,ITP1)= -GTB(I,ITP1)*TTB(ITP1,I) +HF(I)*1000.
      HTB(I,IT)=(HTB(I,IT)+HF(I))*1000.
      HTB(I,ITP1)=(HTB(I,ITP1)+ HF(I))*1000.
10  CONTINUE
      IF(WTMOLE(I)-1.0) 1972,1991,1991
1972 IECC=I
1991 CONTINUE
C
C   MODIFICATIONS FOR LAPP/ARC INTERFACE PROGRAM
C
      WRITE(NUNITD,333) (TITLE(I),I=1,10)
C
C   IDENTIFY LAPP SPECIES IN THE ARCTABLE
C
C   TABLE=SPECIES NAMES AS FOUND IN ARCTABLE
C   15=NUMBER OF SPECIES IN ARCTABLE
C   IZSPEC=NUMBER OF LAPP SPECIES FOUND IN ARCTABLE
C
      M=0
      DO 3 I=1,NS
      DO 3 J=1,16
      IF(AID(I).NE.TABLE(J)) GO TO 3
      M=M+1
      ZSPEC(M)=AID(I)
      ISPEC(M)=I
3  CONTINUE
      IZSPEC=M
      WRITE(NUNITD,334) IZSPEC
334 FORMAT(8I10)
      WRITE(NUNITD,333) (ZSPEC(M),M=1,IZSPEC)
      WRITE (NUNITD,102) THOT,TCOOL
      WRITE(NUNITD,1000) RJ
      DO 301 J = 1,6
      DO 301 I = 1,NS
      IF(AID(I).EQ.XAME(J)) ISAVE(J) = I
301 CONTINUE
      DO 1992 I=1,NR
      READ (NUNITB,444)(ZID(J),J=1,5),IRR(I),IRT(I),(RC(I,K),K=1,3)
      IF(NUNITM.LT.0) WRITE(NNOUT,444)(ZID(J),J=1,5),IRR(I),IRT(I),
      *(RC(I,K),K=1,3)
      DO 1993 J=1,5
      IRRR(I,J)=0
      DO 1993 L=1,NS
      IF(ZID(J)-AID(L)) 1993,1994,1993
1994 IRRR(I,J)=L
1993 CONTINUE
1992 CONTINUE
      DO 912 I=1,MPSI
      WTVR=0.0
      DO 632 J=1,NS

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632 WTVR=WTVR+ALPHA(J,I)*WTMOLE(J)
DO 633 J=1,NS
633 ALPHA(J,I)=ALPHA(J,I)/WTVR
912 CONTINUE
IF(DELPSEI) 903,3041,903
3041 DUM=0.0
DO 5001 J=1,NS
5001 DUM=DUM+ALPHA(J,1)
XMD=MMOD-1
DELPSEI=SQRT(P*U(1)/42.285E0/T(1)/DUM)*RJ/XMD
903 DO 20 I=1,29
XI=I-1
PSI(I)=XI*DELPSEI
XLE(I)=XLE(1)
20 SIGMA(I)=SIGMA(1)
DO 90 I=NPSI,29
RT(I)=T(MPSI)
T(I)=T(MPSI)
DO 80 J=1,NS
RALPHA(J,I)=ALPHA(J,MPSI)
80 ALPHA(J,I)=ALPHA(J,MPSI)
RU(I)=U(MPSI)
90 U(I)=U(MPSI)
IF(NOUT.GT.0)CALL INOUT
PPUNCH = P
P=2117.0*P
DPDX=0.0

C
C PRESSURE OPTION, IF IPRESS= 0, PRESSURE
C IS CONSTANT AND = TO P, IF IPRESS = 1, COEFFICIENTS CALLED
C PC(1),PC(2),PC(3),PC(4) ARE INPUT.
C EQUATION USED IS  $P = PC(1) + PC(2)*X + PC(3)*X*X + PC(4)*X*X*X$ 
C
2 IF(IPRESS) 821,822,821
821 P=(PC(1)+X*(PC(2)+X*(PC(3)+X*PC(4))))*2117.0
DPDX=(PC(2)+X*(2.0*PC(3)+X*3.0*PC(4)))*2117.0
PPUNCH = P/2117.0
822 DO 31 I=1,MPSI
WTMIX(I)=0.0
DO 30 J=1,NS
30 WTMIX(I)=WTMIX(I)+ALPHA(J,I)
RHO(I)=P/89517.501/T(I)/WTMIX(I)
31 RHOOUT(I)=RHO(I)/1.94
DO 805 I=1,MPSI

C
C FREE STREAM VELOCITY WILL BE SET TO 1.0 FPS IF ZERO IS ENTERED
C
U(I) = AMAX1(1.0E0,U(I))
TFDG(I)=AMAX1(T(I),100.00E0)
T4(I)=TFDG(I)**4
XLT(I)=ALOG(TFDG(I))
CPBAR(I)=0.0
HSTAT(I)=0.0
TX=T(I)
DO 805 J=1,NS

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      JJ=J
      CALL TKEY (TX,TTB,ITKEY,SDT,HDT,NT,JJ)
      IF (ITKEY.EQ.0) GO TO 9
      CP(J,I)=0.0
      H(J,I)=0.0
      CALL LIPLN(ITKEY,J,CPTB,SDT,HDT,AX)
      CP(J,I)=AX*45055.31
      CALL LIPLN(ITKEY,J,HTB,SDT,HDT,AX)
      H(J,I)=AX*45055.31
      HSTAT(I)=HSTAT(I)+H(J,I)*ALPHA(J,I)
805 CPBAR(I)=CPBAR(I)+CP(J,I)*ALPHA(J,I)
      ETA(1)=0.0
      Y(1)=0.0
C*****CALL
      ETA(2)=DELPSI/SQRT(RHO(1)*U(2))
      Y(2)=DELPSI/SQRT(RHO(2)*U(2))
      DO 25 I=3,MPSI
      ETA(I)=SQRT(ETA(I-2)**2+DELPSI*(PSI(I)/U(I)+4.0E0*PSI(I-1)/U(I-1)
1+PSI(I-2)/U(I-2))/1.5/RHO(1))
      TEMP = (Y(I-2)**2+DELPSI*(PSI(I)/RHO(I)/U(I)+4.0*PSI(I-1)/RHO(I-1)
1 /U(I-1)+PSI(I-2)/RHO(I-2)/U(I-2))/1.5)
1003 FORMAT(I5,7E10.3)
      IF(TEMP.LT.0.0) CALL OUTPUT
      Y(I) =SQRT(TEMP)
      25 CONTINUE
C
C**** HAS MIXING REGION INTERSECTED X AXIS YET, YES IF 0 OR -
C
      IF (ITURB-6) 8010,8011,8010
8010 IF (U(1) - USUB01) 9000,9000,9001
C
C      MODEL 6 COMMON CALCULATIONS
C
8011 QQ1 = (U(1)+U(MPSI))/2.0
      DO 8012 I=2,MPSI
      IF ((QQ1-U(I))*(QQ1-U(I-1))) 8013,8013,8012
8012 CONTINUE
8013 QQ2 = (QQ1-U(I-1))/(U(I)-U(I-1))
      QQ100 = Y(I-1)+(Y(I)-Y(I-1))*QQ2
      QQ30 = T(I-1)+(T(I)-T(I-1))*QQ2
      QQ3 = CPBAR(I-1)+(CPBAR(I)-CPBAR(I-1))*QQ2
      QQ4 = 1.0/(WTMIX(I-1)+(WTMIX(I)-WTMIX(I-1))*QQ2)
      QQ5 = 89517.501/QQ4
      QQ6 = QQ3/(QQ3-QQ5)
      QQ7 =SQRT(QQ6*QQ5*QQ30)
      QQ300 = QQ1/QQ7
      QQ8 = (ABS(U(1)-U(MPSI)))/2.0
      IF (QQ300-1.2) 8014,8014,8015
8014 QQ400 = (.0468+QQ300*((QQ300*(-.0460))+.0256*(QQ300*QQ300)))*XK2
      GO TO 8016
8015 QQ400 = .0248*XK2
8016 IF ((U(1)-USUB01)*(U(1)-U(MPSI))) 8020,8020,8800
8020 IF (USUB01-9000.0) 8021,8021,8900
8021 USUB01 = 10000.0

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      XDUM=X*0.3048
      WRITE(NOUT,9900) XDUM
      GO TO 8900
C
C      MODEL 6 BEFORE MIXING ZONE REACHES AXIS
C
      8800 QQ9 = 0.95* (U(1)-U(MPSI)) + U(MPSI)
      DO 8802 I = 2,MPSI
      IF ((QQ9-U(I))*(QQ9-U(I-1))) 8804,8804,8802
      8802 CONTINUE
      8804 QQ200 = Y(I-1)+(Y(I)-Y(I-1))*(QQ9-U(I-1))/(U(I)-U(I-1))
      QQ10 = QQ400*QQ8*(QQ100-QQ200)
      DO 8810 I = 1,MPSI
      8810 XMU(I) = QQ10*RHO(I)
      GO TO 98
C
C      MODEL 6 AFTER MIXING ZONE REACHES AXIS
C
      8900 QQ11 = QQ400*QQ100*QQ8
      DO 8910 I = 1,MPSI
      8910 XMU(I) = QQ11*RHO(I)
      QQ200 = 0.0
      GO TO 98
      9000 IQ77 = 9
      USUB01 = 0.0
      WRITE(NOUT,9900)X
      9001 LL = ITURB + IQ77
C
C      EDDY VISCOSITY MODELS
C
      GO TO (91,99,8666,78,8667,8668,9003,91,99,45,78,26,33,78),LL
C
C      MODEL 1 BEFORE MIXING ZONE REACHES AXIS
C
      8666 XMU(1)=0.00137*(X+1.0E-05)*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))
      GO TO 37
C
C      MODEL 3 BEFORE MIXING ZONE REACHES AXIS
C
      8667 XMU(1)=0.00137*(X+1.0E-05)*RHO(1)*ABS(U(1)-U(MPSI))
      GO TO 37
C
C      MODEL 4 BEFORE MIXING ZONE REACHES AXIS
C
      8668 XMU(1)=0.00137*(X+1.0E-05)*RHO(MPSI)*ABS(U(1)-U(MPSI))
      GO TO 37
      91 DO 92 I=1,MPSI
C
C      MODEL 0 LAMINAR FLOW
C
      92 XMU(I)=3.05E-8*T(I)**1.5/(T(I)+111.0)
      GO TO 98
      45 DUM=.5*(RHO(1)*U(1)+RHO(MPSI)*U(MPSI))
      DO 52 J=1,MPSI

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      I=MPSI-J+1
      IF(RHO(I)*U(I)-DUM) 52,52,51
52  CONTINUE
C
C      MODEL 1 AFTER MIXING ZONE REACHES AXIS
C
51  Z=Y(I)+(Y(I)-Y(I+1))*(RHO(I)*U(I)-DUM)/(RHO(I)*U(I)-RHO(I+1)*U(I+1))
      XMU(1)=XK2*Z*ABS(RHO(1)*U(1)-RHO(MPSI)*U(MPSI))*0.025
      GO TO 37
99  DO 39 I=1,MPSI
39  XMU(I)=XK2*0.025
      GO TO 98
78  RD=(U(1)+U(MPSI))/2.0
      DO 47 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 48,48,47
47  CONTINUE
48  RHALVE=ETA(I-1)+(ETA(I)-ETA(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
      DUMMY=XK2*RHALVE*ABS(U(1)-U(MPSI))*0.025
      XMU(1)=DUMMY*RHO(1)
      DO 79 I=2,MPSI
C
C      MODEL 2 BEFORE MIXING ZONE REACHES AXIS
C
79  XMU(I)=DUMMY*(RHO(1)*ETA(I)/Y(I))**2/RHO(I)
      GO TO 98
C
C      MODEL 2 AFTER MIXING ZONE REACHES AXIS
26  RD=(U(1)+U(MPSI))/2.0
      DO 27 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 28,28,27
27  CONTINUE
28  RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
C
C      MODEL 3 AFTER MIXING ZONE REACHES AXIS
C
      XMU(1)=XK2*RHALVE*RHO(1)*ABS(U(1)-U(MPSI))*0.025
      DO 29 I=1,MPSI
29  XMU(I)=XMU(1)
      GO TO 98
33  RD=(U(1)+U(MPSI))/2.0
      DO 34 I=2,MPSI
      IF ((RD-U(I))*(RD-U(I-1))) 35,35,34
34  CONTINUE
35  RHALVE=Y(I-1)+(Y(I)-Y(I-1))*(RD-U(I-1))/(U(I)-U(I-1))
C
C      MODEL 4 AFTER MIXING ZONE REACHES AXIS
C
      XMU(1)=XK2*RHALVE*RHO(MPSI)*ABS(U(1)-U(MPSI))*0.025
37  DO 36 I=1,MPSI
36  XMU(I)=XMU(1)
      GO TO 98
C
C      MODEL 5 BEFORE MIXING ZONE REACHES AXIS
C
9003 XMU(1) = 0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*RHO(1)

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      DO 9004 I = 2,MPSI
      XMU(I)=0.00137*(X+1.0E-05)*ABS(UNIT-U(MPSI))*(RHO(1)**2/RHO(I))
9004  CONTINUE
      98  A(1)=0.0
C
C      CALCULATE A
C
      DO 44 I=2,MPSI
44  A(I)=XMU(I)*RHO(I)*U(I)*Y(I)*Y(I)/PSI(I)
      DO 899 L=1,NPSI
      RRT=1.986*T(L)
      ROOTT=SQRT(T(L))
      TX=T(L)
      DO 855 I=1,NS
      II=I
      CALL TKEY(TX,TTB,ITKEY,SDT,HDT,NT,II)
      IF (ITKEY.EQ.0) GO TO 9
      G(I)=0.0
      WP(I)=0.0
      WM(I)=0.0
      QX(I,L)=0.0
      DO 872 J=1,NS
872  CM(I,J,L)=0.0
      CALL LIPLN(ITKEY,I, GTB,SDT,HDT,AX)
      G(I)=AX
855  CONTINUE
C
C      REACTION CALCULATION
C      REACTION KINETICS CONTINUE DOWN TO 400 DEGREES K
C      UNLESS TKINET IS SET TO A VALUE OTHER THAN 400 K
C      REACTION KINETICS FOR ALL REACTIONS CONTINUE DOWN TO TKINET
C
      IF(T(L)-TKINET) 3256,3256,3259
3259  CONTINUE
      DO 862 I=1,NR
      RP(I,L)=0.0
      RM(I,L)=0.0
      KK = IRT(I)
C
C      REACTION CONSTANT TYPE
C
      GO TO (841,842,843,844,845,846,847),KK
841  RATE=RC(I,1)*AV
      GO TO 849
842  RATE=RC(I,1)/T(L)*AV
      GO TO 849
843  RATE=RC(I,1)/T(L)/T(L)*AV
      GO TO 849
844  RATE=RC(I,1)/ROOTT*AV
      GO TO 849
845  RATE=RC(I,1)*EXP(RC(I,3)/RRT)*AV
      GO TO 849
846  RATE=RC(I,1)*EXP(RC(I,3)/RRT)/T(L)**RC(I,2)*AV
      GO TO 849
847  RATE=RC(I,1)/T(L)/ROOTT*AV

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849 CONTINUE
    K=IRR(I)
C
C    TYPE OF REACTION
C
    GO TO(864,865,866,870,871,834,835,836,837,838),K
870 J1=IRRR(I,1)
    J2=IRRR(I,2)
    J3=IRRR(I,3)
    E = (G(J1)+G(J2)-G(J3))/RRT
    IF(ABS(E).LT.80.0) GO TO 700
    IF(E.LT.0.0) E=EXP(-80.0E0)
    IF(E.GT.0.0) E =EXP(80.0E0)
    GO TO 701
700 E =EXP(E)
701 CONTINUE
    CRR=RATE*RHOOUT(L)
    RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
    RM(I,L)=CRR*ALPHA(J3,L)/E/R/T(L)
    DO 771 J=1, 3
    SIGN=1.0
    IF (J.GT.2) SIGN=-1.0
    IROW= IRRR(I,J)
    CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
    CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
    CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
771 QX(IROW,L)= QX(IROW,L)+ SIGN*RP(I,L)
    GO TO 868
871 J1=IRRR(I,1)
    J2=25
    J3=IRRR(I,3)
    J4=IRRR(I,4)
    E = (G(J1)-G(J3)-G(J4))/RRT
    IF(ABS(E).LT.80.0) GO TO 702
    IF( E.LT.0.0) E =EXP(-80.0E0)
    IF( E.GT.0.0) E =EXP(80.0E0)
    GO TO 703
702 E =EXP(E)
703 CONTINUE
    CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)
    RP(I,L)=CRR*ALPHA(J1,L)
    RM(I,L)=CRR*R*T(L)*RHOOUT(L)*ALPHA(J3,L)*ALPHA(J4,L)/E
    DO 772 J=1, 4
    SIGN=1.0
    IF (J.GT.2) SIGN=-1.0
    IROW= IRRR(I,J)
    IF(J.EQ.2) IROW=25
    CM(IROW,J1,L)= CM(IROW,J1,L)+SIGN*CRR
    CM(IROW,J3,L)= CM(IROW,J3,L)-SIGN*RM(I,L)/ALPHA(J3,L)
    CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
772 QX(IROW,L)= QX(IROW,L)- SIGN*RM(I,L)
    GO TO 867
864 J1=IRRR(I,1)
    J2=IRRR(I,2)
    J3=IRRR(I,3)

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J4=IRRR(I,4)
E = (G(J1)+G(J2)-G(J3)-G(J4))/RRT
IF(ABS(E).LT.80.0) GO TO 704
IF(E.LT.0.0) E =EXP(-80.0E0)
IF(E.GT.0.0) E =EXP(80.0E0)
GO TO 705
704 E = EXP(E)
705 CONTINUE
    CRR=RATE*RHOOUT(L)*RHOOUT(L)
    RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
    RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)/E
    DO 773 J=1, 4
    SIGN=1.0
    IF (J.GT.2) SIGN=-1.0
    IROW= IRRR(I,J)
    CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
    CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
    CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
    CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
773 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-RM(I,L))
    GO TO 867
865 J1=IRRR(I,1)
    J2=IRRR(I,2)
    J3=IRRR(I,3)
    E = (G(J1)+G(J2)-G(J3))/RRT
    IF(ABS(E).LT.80.0) GO TO 706
    IF(E.LT.0.0) E=EXP(-80.0E0)
    IF(E.GT.0.0) E=EXP(80.0E0)
    GO TO 707
706 E =EXP(E)
707 CONTINUE
    CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV
    RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
    RM(I,L)=CRR*ALPHA(J3,L)/(E*R*T(L))
    DO 774 J=1,3
    SIGN=1.0
    IF (J.GT.2) SIGN=-1.0
    IROW= IRRR(I,J)
    CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
    CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
    CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
774 QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L) )
    GO TO 868
866 J1=IRRR(I,1)
    J2=IRRR(I,2)
    J3=IRRR(I,3)
    J4=IRRR(I,4)
    J5=IRRR(I,5)
    E = (G(J1)+G(J2)-G(J3)-G(J4)-G(J5))/RRT
    IF(ABS(E).LT.80.0E0) GO TO 708
    IF(E.LT.0.0) E=EXP(-80.0E0)
    IF(E.GT.0.0) E =EXP(80.0E0)
    GO TO 709
708 E =EXP(E)
709 CONTINUE

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```

      CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=CRR*ALPHA(J3,L)*ALPHA(J4,L)*ALPHA(J5,L)*RHOOUT(L)*R*T(L)/E
      DO 775 J=1, 5
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
      CM(IROW,J3,L)= CM(IROW,J3,L) -SIGN*RM(I,L)/ALPHA(J3,L)
      CM(IROW,J4,L)= CM(IROW,J4,L)-SIGN*RM(I,L)/ALPHA(J4,L)
      CM(IROW,J5,L)= CM(IROW,J5,L)-SIGN*RM(I,L)/ALPHA(J5,L)
775  QX(IROW,L)= QX(IROW,L)+ SIGN*(RP(I,L)-2.*RM(I,L))
      GO TO 861
837  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      CRR=RATE*RHOOUT(L)
      RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=0.0
      DO 776 J=1, 3
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
776  QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
      GO TO 868
838  J1=IRRR(I,1)
      J2=25
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)
      RP(I,L)=CRR*ALPHA(J1,L)
      RM(I,L)=0.0
      DO 777 J=1, 4
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      IF (J.EQ.2) IROW=25
777  CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*CRR
      GO TO 867
834  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      CRR=RATE*RHOOUT(L)*RHOOUT(L)
      RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
      RM(I,L)=0.0
      DO 778 J=1, 4
      SIGN=1.0
      IF (J.GT.2) SIGN=-1.0
      IROW= IRRR(I,J)
      CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
      CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)

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778 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
GO TO 867
835 J1=IRRR(I,1)
J2=IRRR(I,2)
J3=IRRR(I,3)
CRR=RATE*RHOOUT(L)*RHOOUT(L)*WTMIX(L)*AV
RP(I,L)=CRR*RHOOUT(L)*ALPHA(J1,L)*ALPHA(J2,L)
RM(I,L)=0.0
DO 779 J=1, 3
SIGN=1.0
IF (J.GT.2) SIGN=-1.0
IROW= IRRR(I,J)
CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
779 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
GO TO 868
836 J1=IRRR(I,1)
J2=IRRR(I,2)
J3=IRRR(I,3)
J4=IRRR(I,4)
J5=IRRR(I,5)
CRR=RATE*RHOOUT(L)*RHOOUT(L)
RP(I,L)=CRR*ALPHA(J1,L)*ALPHA(J2,L)
RM(I,L)=0.0
DO 780 J=1, 5
SIGN=1.0
IF (J.GT.2) SIGN=-1.0
IROW= IRRR(I,J)
CM(IROW,J1,L)= CM(IROW,J1,L) +SIGN*RP(I,L)/ALPHA(J1,L)
CM(IROW,J2,L)= CM(IROW,J2,L) +SIGN*RP(I,L)/ALPHA(J2,L)
780 QX(IROW,L)= QX(IROW,L)+ SIGN* RP(I,L)
C
C CALCULATE WDOT
C
861 WP(J5)=WP(J5)+RP(I,L)
WM(J5)=WM(J5)+RM(I,L)
867 WP(J4)=WP(J4)+RP(I,L)
WM(J4)=WM(J4)+RM(I,L)
868 WP(J3)=WP(J3)+RP(I,L)
WM(J3)=WM(J3)+RM(I,L)
WP(J2)=WP(J2)+RM(I,L)
WM(J2)=WM(J2)+RP(I,L)
WP(J1)=WP(J1)+RM(I,L)
WM(J1)=WM(J1)+RP(I,L)
862 CONTINUE
3256 CONTINUE
DO 897 J=1, NS
897 WDOT(J,L)=(WP(J)-WM(J))/RHOOUT(L)/U(L)
899 CONTINUE
IOUT=IOUT+1
63 IF(IFINIS) 65,69,65
65 IF(X-XMAX) 67,66,66
67 IF(PRNT-PCNT) 69,69,68
68 CONTINUE
GO TO 5

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66 IFINIS=2
69 CALL OUTPUT
   PCNT=0.0
   IF(IFINIS-1) 5,5,6
C
C   CHECK DIFFUSION STEP SIZE
C
5 XD=DELPSI*DELPSI*SIGMA(1)/XMU(1)/XLE(1)/12.0 *FDL
  DO 511 I=2,NPSI
    DUMMY=A(I+1)+A(I-1)+A(I)+A(I)
    DUMMY=PSI(I)*DELPSI*DELPSI*SIGMA(I)/XLE(I)/DUMMY/1.5*FDL
511 XD=AMIN1(XD,DUMMY)
    DX=AMIN1(DX,XD)
    DO 101 I=2,NPSI
      EX1=PSI(I)*DELPSI**2/DX
      EX11=.5*(A(I)+A(I+1))
      EX12=.5*(A(I)+A(I-1))
C
C   INTEGRATE MOMENTUM EQUATION
C
RU(I)=(EX11*(U(I+1)-U(I))+EX12*(U(I-1)-U(I)))/EX1+U(I)
RU(I)=RU(I)-DX*DPDX/RHO(I)/U(I)
EX3=0.0
EX4=0.0
DO 21 J=1,NS
  EX3=EX3+H(J,I)*WDOT(J,I)
21 EX4=EX4+CP(J,I)*(ALPHA(J,I+1)-ALPHA(J,I-1))
  EX2=EX1*CPBAR(I)
  EX5=XLE(I)*A(I)/SIGMA(I)
  EX6=.5*(EX5+XLE(I+1)*A(I+1)/SIGMA(I+1))
  EX7=.5*(EX5+XLE(I-1)*A(I-1)/SIGMA(I-1))
  EX8=CPBAR(I)*A(I)/SIGMA(I)
  EX9=.5*(EX8+CPBAR(I+1)*A(I+1)/SIGMA(I+1))
  EX10=.5*(EX8+CPBAR(I-1)*A(I-1)/SIGMA(I-1))
  EX14=EX4*EX5/4.0
C
C   INTEGRATE ENERGY EQUATION
C
RT(I)=(U(I+1)-U(I-1))**2*A(I)/EX2/4.0+DX*DPDX/RHO(I)/CPBAR(I)+T(I)
1+(EX9+EX14)*T(I+1)+(EX10-EX14)*T(I-1)-(EX9+EX10)*T(I))/EX2-EX3*DX
2/CPBAR(I)
RHOUIX=DX/(RHOOUT(I)* U(I))
C
C   INTEGRATE SPECIES EQUATIONS
C
DO 41 J=1,NS
41 QX1(J) =(EX6*(ALPHA(J,I+1)-ALPHA(J,I))+EX7*(ALPHA(J,I-1)-ALPHA
1(J,I)))/EX1+ALPHA(J,I)+ QX(J,I)*RHOUIX
  DO 781 M=1,NS
    DO 781 N=1,NS
      CM1(M,N)= CM(M,N,I)*RHOUIX
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0
781 CONTINUE
  CALL SLDP(QX1,CM1,NS)
785 FORMAT (1H , 2I5)

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      DO 782 J=1, NS
782  RALPHA(J,I)= QX1(J)
101  CONTINUE
      EX3=4.0*XMU(1)*DX/DELPsi/DELPsi
      RHOUIX=DX/(RHOOUT(1)* U(1))
C
C      COMPUTE U AT CENTER LINE
C
      RU(1)=EX3*(U(2)-U(1))+U(1)-DX*DPDX/RHO(1)/U(1)
      EX4=0.0
      DO 200 J=1,NS
      EX4=EX4+H(J,1)*WDOT(J,1)
      RALPHA(J,MPSI)=ALPHA(J,MPSI)
200  QX1(J) =EX3*XLE(1)*(ALPHA(J,2)-ALPHA(J,1))/SIGMA(1)+ALPHA(J,1)
      1+ QX(J,1)*RHOUIX
      DO 783 M=1,NS
      DO 783 N=1,NS
      CM1(M,N)= CM(M,N,1)*RHOUIX
      IF (M.EQ.N) CM1(M,N)=CM1(M,N) +1.0
783  CONTINUE
      CALL SLDP(QX1,CM1,NS)
      DO 784 J=1, NS
C
C      COMPUTE SPECIES AT CENTER LINE
C
784  RALPHA(J,1)= QX1(J)
C
C      CALCULATE TEMP. AT CENTER LINE
C
      RT(1)=EX3*(T(2)-T(1))/SIGMA(1)+T(1)+DX*DPDX/RHO(1)/CPBAR(1)
      1-EX4*DX/CPBAR(1)
      RT(MPSI)=T(MPSI)
      IF(IEDGE) 230,231,230
C
C      COMPUTE TEMP. AND U AT EDGE
C
230  RU(MPSI)=U(MPSI)-DX*DPDX/RHO(MPSI)/U(MPSI)
      RT(MPSI)=T(MPSI)+DX*DPDX/RHO(MPSI)/CPBAR(MPSI)
      DO 210 I=MPSI,29
      RU(I)=RU(MPSI)
      U(I)=RU(MPSI)
      RT(I)=RT(MPSI)
210  T(I)=RT(MPSI)
231  CONTINUE
      1 IFINIS=1
921  SAVEX=X
      SAVEDX=DX
      DO 941 I=1,29
      SAVEU(I)=U(I)
      SAVET(I)=T(I)
      DO 940 J=1,NS
      SAVEA(J,I)=ALPHA(J,I)
940  CONTINUE
941  CONTINUE
      MINIT = 13

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      MHALF = 25
      NTEST=MPSI-1
      DO 967 I=1,NTEST
C
C      CHECK NEGATIVE MOLE FRACTION
C
965 DO 967 J=1,NS
      IF (RALPHA(J,I)) 995,967,967
967 CONTINUE
      X=X+DX
      PCNT=PCNT+DX
      DX=XD
      DO 925 I=1,29
      DO 926 J=1,NS
926 ALPHA(J,I)=RALPHA(J,I)
      T(I)=RT(I)
925 U(I)=RU(I)
      GO TO 999
995 IF (DX.LT.DXMIN) GO TO 8000
981 DX=SAVEDX/2.0
      X=SAVEX
      DO 985 I=1,29
      DO 982 J=1,NS
982 ALPHA(J,I)=SAVEA(J,I)
      T(I)=SAVET(I)
985 U(I)=SAVEU(I)
      GO TO 2
C
C      IF MPSI .GE.26 ,MPSI IS HALVED
C
999 IF(MPSI-MHALF) 1001,1500,1500
1001 IF(ABS(U(NPSI)-U(MPSI))/U(MPSI)-.010E0) 1011,1011,1004
1011 IF(ABS(T(NPSI)-T(MPSI))/T(MPSI)-.050E0) 1002,1002,1004
1002 CONTINUE
      GO TO 2000
1004 MPSI=MPSI+1
      NPSI=MPSI-1
      DO 1101 I=MPSI,29
      SAVEU(I)=U(NPSI)
      RU(I)=U(NPSI)
      U(I)=U(NPSI)
      SAVET(I)=T(NPSI)
      T(I)=T(NPSI)
      RT(I)=T(NPSI)
      DO 1102 J=1,NS
      SAVEA(J,I)=ALPHA(J,NPSI)
      ALPHA(J,I)=ALPHA(J,NPSI)
1102 RALPHA(J,I)=ALPHA(J,NPSI)
1101 CONTINUE
      GO TO 2000
1500 IFINIS=0
      DELPSI=DELPSI+DELPSI
      DO 1600 I=1,MINIT
      DO 1650 J=1,NS
1650 ALPHA(J,I)=ALPHA(J,2*I-1)

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      T(I)=T(2*I-1)
1600 U(I)=U(2*I-1)
      MPSI=MINIT
      NPSI=MPSI-1
      DO 1700 I=MINIT,29
      DO 1750 J=1,NS
      ALPHA(J,I)=ALPHA(J,MPSI)
1750 RALPHA(J,I)=ALPHA(J,MPSI)
      T(I)=T(MPSI)
      RT(I)=T(MPSI)
      U(I)=U(MPSI)
1700 RU(I)=U(MPSI)
      DO 1800 I=2,29
1800 PSI(I)=PSI(I-1)+DELPSI
      ITER=0
      ISTEP=0
      GO TO 2000
8000 WRITE(NDBG,8001)
8001 FORMAT(68H1NEGATIVE PARAMETER - NOT CORRECTED BY REPEATED HALVING
      1OF STEP SIZE)
      IFINIS=2
      GO TO 69
2000 CONTINUE
      CALL TICK(ISECS)
      IELAPS = ISECS-ISECST
      IF(IELAPS.LT.0) IELAPS = IDIFFT + ISECS
      IF(IELAPS.GE.ILIMIT) GO TO 6
      GO TO 2
100 FORMAT(14I5)
102 FORMAT(8F10.4)
111 FORMAT (7( E10.3))
222 FORMAT(A6,7E10.3)
333 FORMAT(10A8)
444 FORMAT(A6,1X,A6,8X,A6,1X,A6,1X,A6,7X,I2,I1,E8.2,F4.1,F9.1)
555 FORMAT(8( E10.3))
666 FORMAT(10I5)
1000 FORMAT(7E10.3)
9900 FORMAT (39H1 MIXING REGION INTERSECTS AXIS AT X = E15.7)
6 CONTINUE
      XORJ=X/RJ
790 FORMAT( E10.3,60X,E10.3)
      IF (IPUNCH .EQ. 0 .OR. IPUNCH .EQ. 1) GO TO 9
      X=X*AMULT
      XMAX=XMAX*AMULT
      PRNT=PRNT*AMULT
      RJ=RJ*AMULT
      DXMIN=DXMIN*AMULT
      PC(2)=PC(2)/AMULT
      PC(3)=PC(3)/AMULT1
      PC(4)=PC(4)/AMULT2
      DELPSI=DELPSI*AMULT3
      DO 7666 I=1,MPSI
7666 U(I)=U(I)*AMULT
      WRITE(NUNITE,333)(TITLE(I),I=1,10)
      WRITE(NUNITE,666)MPSI,NS,ITURB,NR,IOUT1,IOUT2,IPUNCH,ITIME,

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*IPRESS,NT
WRITE(NUNITE,1000)FREQA(1),FREQA(2),FREQA(3),FREQA(4),FREQA(5),
*FREQA(6)
WRITE(NUNITE,1000) X,XMAX,PRNT,XLE(1),SIGMA(1),RJ,XK2
WRITE(NUNITE,1000) DXMIN, FDL, PC(1),PC(2),PC(3),PC(4)
WRITE(NUNITE,1000) PPUNCH,T(1),T(MPSI),U(1),U(MPSI),DELPSI,TKINET
WRITE(NUNITE,1000) (T(I),I=1,MPSI)
WRITE(NUNITE,1000) (U(I),I=1,MPSI)
DO 8 I = 1,MPSI
DO 1104 J=1,NS
1104 RALPHA(J,I)=RALPHA(J,I)/WTMIX(I)
WRITE(NUNITE,1000) (RALPHA(J,I),J=1,NS)
8 CONTINUE
9 CONTINUE
STOP
END
SUBROUTINE OUTPUT
DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
2 WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),
3RU(30),U(30),TITLE(12),XLE(30),XMU(30),G(25),WTMIX(30),
4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),
5 IRR(49),FREQ(30),SAVEA(25,30),PC(4),ZID(5),
6 ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),
7T4(30),TFDG(30),IRT(49),RP(49,30),RM(49,30)
DIMENSION ISAVE(6), FREQA(6), ALOC(50,6), ATT(6), YATT(50)
DIMENSION ZCON(16,30)
COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
COMMON/UNITS/NUNITA,NUNITB,NUNITC,NUNITD,NUNITE,NUNITF,
*NUNITG,NUNITH,NUNITI,NUNITJ,NUNITK,NUNITL,NUNITM,NUNITN,
*NOUT,NDBG,NNNOUT
COMMON/C/ IZSPEC,ISPEC(16)
COMMON A , RHO , Y , T , PSI , RT
COMMON SUM , AR , HSTAT , H , ALPHA , RALPHA
COMMON CP , SIGMA , WTMOLE , CPBAR , C
COMMON AID , ETA , RATIO , RU , U , TITLE
COMMON XLE , XMU , G , WTMIX , WDOT
COMMON SAVEU , SAVET , WM , WP , RC
COMMON SAVEA , PC , X , XMAX
COMMON PRNT , DXMIN , DX , FDL , DELPSI , RJ
COMMON XK2 , P , ZID , FREQ , ECC , DPDX
COMMON Y OUT , HOUT , RHOOUT , IRRR , IRR , IFINIS
COMMON IPAGE , MPSI , MY , NS , NR , IEDGE
COMMON ITURB , IPRESS , NPSI , ITEST , ITER , IECC
COMMON IRT , XMU OUT , XLT , T4 , TFDG , IOUT
COMMON IOUT1 , IOUT2 , RP , RM , ISAVE , IPUNCH
COMMON TKINET,NFREQA,ALOC,FREQA,QQ100,QQ200,QQ300,QQ400
DATA AMULT5/1000./,AMULT4/1.488/
DATA BLANK/8H /
DATA ZCO /6HCO /
DATA ZCO2/6HCO2 /
DATA ZH2O/6HH2O /
DATA ZO /6HO /
DATA ZOH/6HOH /
DATA ZAL/6HAL2O3 /

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```

DUMMY = 0.0
BIG=1.0E30
NS1=NS+1
IF(NS1 .GT. 25) GO TO 2
DO 1 I=NS1,25
1  AID(I)=BLANK
2  DO 5 I=1, NS
    IF (AID(I).EQ.ZCO ) ICO =I
    IF (AID(I).EQ.ZCO2) ICO2=I
    IF (AID(I).EQ.ZH2O) IH2O=I
    IF (AID(I).EQ.ZO ) IO =I
    IF (AID(I).EQ.ZOH) IOH=I
    IF (AID(I).EQ.ZAL) IAL=I
5  CONTINUE
    IF(IECC) 531,539,531
531 DO 532 I=1,MPSI
532 ECC(I)=RHO(I)*ALPHA(IECC,I)*3.108E23
539 DO 10 I=1,MPSI
    YOUT(I)=Y(I)/RJ
    XMUOUT(I)=XMU(I)*32.174
    HOUT(I)=HSTAT(I)/45055.31
    SUM(I)=0.0
    DO 10 J=1,NS
10  SUM(I)=SUM(I)+ALPHA(J,I)*WTMOLE(J)
    UD=.05*U(1)+.95*U(MPSI)
    DO 83 I=2,MPSI
    IF ((U(I)-UD)*(U(I-1)-UD)) 84,84,83
83  CONTINUE
84  VR=(Y(I)-Y(I-1))*(UD-U(I-1))/(U(I)-U(I-1))+Y(I-1)
    TD=.05*T(1)+.95*T(MPSI)
    DO 85 I=2,MPSI
    IF ((T(I)-TD)*(T(I-1)-TD)) 86,86,85
85  CONTINUE
86  TR=(Y(I)-Y(I-1))*(TD-T(I-1))/(T(I)-T(I-1))+Y(I-1)
    TR=TR/RJ
    VR=VR/RJ
    DO 87 J=1,NS
    AR(J)=0.0
    AD=.05*ALPHA(J,1)+.95*ALPHA(J,MPSI)
    IF(ALPHA(J,MPSI)) 91,92,91
91  DO 88 I=1,MPSI
    IF(ALPHA(J,I)-AD) 88,88,89
88  CONTINUE
89  AR(J)=Y(I-1)+(Y(I)-Y(I-1))*(AD-ALPHA(J,I-1))/(ALPHA(J,I)-ALPHA(J,I
    1-1))
    AR(J)=AR(J)/RJ
    GO TO 87
92  DO 93 I=1,MPSI
    IF(ALPHA(J,I)-AD) 94,93,93
93  CONTINUE
94  GO TO 89
87  CONTINUE
    PCNT=0.0
    IPAGE=IPAGE+1
    XXOUT=X*AMULT

```

```

XXX=XXOUT
WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
WRITE (NOUT,102)
XORJ=X/RJ
POUT=P/2117.0
DPOUT=DPDX/2117.0
DDX=DX*AMULT
WRITE(NOUT,103) XORJ,DDX,POUT
IF (ITURB-6) 8600,8500,8600
8500 WRITE (NOUT,8555)
QQ101=QQ100/RJ
QQ201=QQ200/RJ
WRITE (NOUT,8556) QQ101,QQ201,QQ300,QQ400
8555 FORMAT(1H0,8X,4HHALF,21X,12HINNER MIXING,17X,11HMACH NUMBER,16X,11
*H MIXING RATE/7X,10HRADIUS/R ,16X,15HZONE RADIUS/R ,14X,14HAT HAL
*F RADIUS,14X,11HCOEFFICIENT)
8556 FORMAT (4X, E14.6, 3E28.6)
8600 WRITE (NOUT,107)
WRITE (NOUT,509)
TTT=T(1)
WRITE(NNNOUT,8888)XXX,TTT
8888 FORMAT(F6.1,F8.1)
DO 73 I=1,MPSI
SS1= 89517.501*WTMIX(I)
SS2= CPBAR(I)/(CPBAR(I)-SS1)
SS=SQRT(SS2*SS1*T(I))
XMACH= U(I)/SS
UU=U(I)*AMULT
RRHOUT=RHOOUT(I)*AMULT5
XXMOUT=XMUOUT(I)*AMULT4
PPSI=PSI(I)*AMULT3
IF(IECC) 71,72,71
71 WRITE (NOUT,207)I,YOUT(I),UU,T(I),RRHOUT,XMACH, HOUT(I),
*XXMOUT,ECC(I),PPSI,I
GO TO 73
72 WRITE (NOUT,307)I,YOUT(I),UU,T(I),RRHOUT,XMACH, HOUT(I),
*XXMOUT,PPSI,I
73 CONTINUE
DO 581 I=1,MPSI
DO 581 J=1,NS
581 RALPHA(J,I)=ALPHA(J,I)/WTMIX(I)
IRPT=(NS+6)/7
DO 564 KK=1,IRPT
I1=1+(KK-1)*7
I2=7+(KK-1)*7
WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
WRITE (NOUT,409)
IF (I2.GE.25) GO TO 50
WRITE (NOUT,108)(AID(J),J=I1,I2)
DO 81 I=1,MPSI
81 WRITE (NOUT,208)I,YOUT(I),(RALPHA(J,I),J=I1,I2),I
IF(IOUT1)564,564,74
74 WRITE (NOUT,420)
WRITE (NOUT,421)(AID(J),J=I1,I2)
DO 82 I=1,MPSI

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      IF(T(I)-TKINET) 564,564,82
82  WRITE (NOUT,422)I,(WDOT(J,I),J=I1,I2),I
      GO TO 564
50   I2=25
      WRITE (NOUT,108) (AID(J),J=I1,I2)
      DO 52 I=1,MPSI
52  WRITE (NOUT,53) I,YOUT(I),(RALPHA(J,I),J=I1,I2),I
53  FORMAT (I3,F9.5,4E13.5,42X,I3)
      IF (IOUT1) 564,564,54
54  WRITE (NOUT,420)
      WRITE (NOUT,55) (AID(J),J=I1,I2)
55  FORMAT (3H0PT,8X,4(3X,A6,4X),43X,3H PT)
      DO 56 I=1,MPSI
      IF (T(I)-TKINET) 564,564,56
56  WRITE (NOUT,57) I,(WDOT(J,I),J=I1,I2),I
57  FORMAT (I3,9X,4E13.5,42X,I3)
564  CONTINUE
      IF(IOUT2)567,567,75
75  IRPT=(NR+9)/10
      N=0
      NNR=NR-1
      DO 565 KK=1,IRPT
      LL=0
      N=N+1
      WRITE (NOUT,201)XXOUT,(TITLE(I),I=1,10),IPAGE
65  I1=1+(N-1)*5
      I2=5+(N-1)*5
      NNN1=I1
      NNN2=I1+1
      NNN3=I1+2
      NNN4=I1+3
      NNN5=I2
      WRITE(NOUT,209)
      WRITE (NOUT,431)NNN1,NNN2,NNN3,NNN4,NNN5
      WRITE (NOUT,432)
      DO 63 I=1,MPSI
      IF(T(I)-TKINET) 566,566,63
63  WRITE(NOUT,433)I,YOUT(I),(RP(J,I),RM(J,I),J=I1,I2),I
566 IF(NNR/(5*N))565,565,64
64 IF(LL)565,66,565
66 N=N+1
      LL=1
      GO TO 65
565 CONTINUE
567 CONTINUE
568 CONTINUE
1065 CONTINUE
      WRITE (NOUT,1068)
1066 DO 602 I=1,NPSI
      FT1 = 1.0/SQRT(T(I))
      FT2 = 1.0/FT1
      FT3 = 1.0/T(I)
      FT4 = T(I)**0.75
      SUMS = 0.0
      DO 603 IDX = 1,6

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      IF(ISAVE(IDX).EQ.0) GO TO 603
      K = ISAVE(IDX)
      TERM = RALPHA(K,I)
      GO TO (604,605,606,607,608,614),IDX
604  Q = (1.29E-17)*FT2 + 2.46E-16
      GO TO 609
605  Q = (0.758E-13)*FT1
      GO TO 609
606  Q = (1.53E-11)*FT3
      GO TO 609
607  Q = (9.0E-18)*FT2 + 8.9E-16
      GO TO 609
608  Q = 3.29E-23*6.21E5*FT2
      GO TO 609
614  Q= 1.85*(6.21)**(-2)*(1.0E-10)*FT3
609  SUMS = SUMS + Q*TERM
603  CONTINUE
      XNEU = (4.57E27)*SUMS*POUT*FT1
      ECON= 0.07157* ECC(I)/XNEU/.0254
602  IF(IZSPEC.EQ.0) GO TO 613
      WRITE(NUNITD,786) XORJ,MPSI
      DO 615 I=1,MPSI
      YY=Y(I)/RJ
      PP=P/2117.0
      WRITE(NUNITD,785) YY,T(I),PP
      DO 616 M=1,IZSPEC
      K=ISPEC(M)
616  ZCON(M,I)=RALPHA(K,I)
      LINES=IZSPEC/7+1.1
      IF(IZSPEC.EQ.7) LINES=1
      DO 559 L=1,LINES
      LSTART=(L-1)*7+1
      LEND=MIN0(IZSPEC,L*7)
559  WRITE(NUNITD,785) (ZCON(K,I),K=LSTART,LEND)
615  CONTINUE
613  CONTINUE
102  FORMAT(/,8X,3HX/R,8X,14HDELTA X METERS,4X,10HPRESS(ATM))
103  FORMAT(4X, 6E14.6)
107  FORMAT(4H0 PT,5X,3HY/R, 6X,8HVELOCITY,4X,11HTEMPERATURE,5X,7HDENSI
      1TY, 4X8HMACH NO. , 8X,8HENTHALPY,5X,9HVISCOUSITY,
      2 8X,3HPSI,12X,2HPT )
108  FORMAT(103X,3H PT,T1,3H0PT,3X,5H Y/R ,7(3X,A8,2X))
201  FORMAT(1H1,////////3H X= E15.7,7H METERS,8X,10A8,8X,4HPAGEI4)
207  FORMAT(I4,F10.4, 8E14.6,I4)
208  FORMAT(I3,F9.5, 7E13.5,I3)
209  FORMAT(1H ,//40X,28HREACTION RATES (MOLE/ML-SEC)//)
307  FORMAT(I4,F10.4, 7E14.6,4X,I4)
409  FORMAT(1H0,44X,14HMOLE FRACTIONS)
420  FORMAT(1H0,35X,36HNET RATE OF PRODUCTION (W-DOT/RHO*U))
421  FORMAT(3H0PT,8X,7(3X,A6,4X),1X,3H PT)
422  FORMAT(I3,9X, 7E13.5,I3)
431  FORMAT(1H0,2HPT,4X,3HY/R, 8X,5(8HREACTION,I3,11X),2HPT)
432  FORMAT(19X,5(2HRP, 9X,2HRM,10X))
433  FORMAT(I3,1X, 11E11.4,I4)
509  FORMAT(18X,10HMETERS/SEC,4X,10H K ,6X,5HGM/CC,22X,6HCAL/GM,

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      *7X,8HKG/M/SEC)
610 FORMAT(3X,I3,5X,F7.3,8(2X, E10.4))
611 FORMAT(3E15.7)
612 FORMAT(E15.7,I5)
780 FORMAT(8( E10.3))
785 FORMAT(10X,7E10.3)
786 FORMAT(E10.3,I10)
790 FORMAT( E10.3,60X,E10.3)
1068 FORMAT (1H0)
      RETURN
      END
      SUBROUTINE INOUT
      DIMENSION A(30),RHO(30),Y(30),T(30),PSI(30),RT(30),SUM(30),AR(25),
1HSTAT(30),H(25,30),ALPHA(25,30),RALPHA(25,30),CP(25,30),SIGMA(30),
2      WTMOLE(25),CPBAR(30),C(25,9),AID(25),ETA(30),RATIO(30),
3RU(30),U(30),TITLE(12),XLE(30),XMU(30),G(25),WTMIX(30),
4RC(49,3),IRRR(49,5),WP(25),WM(25),WDOT(25,30),SAVET(30),SAVEU(30),
5      IRR(49),FREQ(30),SAVEA(25,30),PC(4),ZID(5),
6      ECC(30),HOUT(30),YOUT(30),RHOOUT(30),XMUOUT(30),XLT(30),
7T4(30),TFDG(30),IRT(49),RP(49,30),RM(49,30)
      DIMENSION ISAVE(6)
      COMMON/CONSTS/AMULT,AMULT1,AMULT2,AMULT3
      COMMON/UNITS/ NNDUM(14),ND,NDBG
      COMMON A , RHO , Y , T , PSI , RT
      COMMON SUM , AR , HSTAT , H , ALPHA , RALPHA
      COMMON CP , SIGMA , WTMOLE , CPBAR , C
      COMMON AID , ETA , RATIO , RU , U , TITLE
      COMMON XLE , XMU , G , WTMIX , WDOT
      COMMON SAVEU , SAVET , WM , WP , RC
      COMMON SAVEA , PC , X , XMAX
      COMMON PRNT , DXMIN , DX , FDL , DELPSI , RJ
      COMMON XK2 , P , ZID , FREQ , ECC , DPDX
      COMMON YOUT , HOUT , RHOOUT , IRRR , IRR , IF INIS
      COMMON IPAGE , MPSI , MY , NS , NR , IEDGE
      COMMON ITURB , IPRESS , NPSI , ITEST , ITER , IECC
      COMMON IRT , XMUOUT , XLT , T4 , TFDG , IOUT
      COMMON IOUT1 , IOUT2 , RP , RM , ISAVE , IPUNCH
      COMMON TKINET

```

C

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      X=X*AMULT
      XMAX=XMAX*AMULT
      PRNT=PRNT*AMULT
      RJ=RJ*AMULT
      DXMIN=DXMIN*AMULT
      DO 7666 I=1,MPSI
7666 U(I)=U(I)*AMULT

```

C

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      WRITE(ND,1901)
      WRITE(ND,1902)
      WRITE(ND,1903)(TITLE(I),I=1,10)
      IF(IPRESS.NE.0) WRITE(ND,1904)P
      IF(IPRESS.EQ.0) WRITE(ND,1905)P
      WRITE(ND,1908)RJ
      WRITE(ND,1909)XLE(1),SIGMA(1)
      WRITE(ND,1966)X,XMAX

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WRITE(ND,1967)PRNT,DXMIN
LL=ITURB+2
GO TO (1991,1999,1945,1978,1926,1933,9950,8000),LL
1991 WRITE(ND,1959)
GO TO 2999
1999 WRITE(ND,1960)XK2
GO TO 2999
1945 WRITE(ND,1961)XK2
GO TO 2999
1978 WRITE(ND,1962)XK2
GO TO 2999
1926 GO TO 2999
1933 GO TO 2999
8000 WRITE(ND,8001)
8001 FORMAT(1H0,22X,30HDONALDSON/GRAY VISCOSITY MODEL)
GO TO 2999
9950 WRITE(ND,9951)XK2
2999 CONTINUE
WRITE(ND,1916)
WRITE(ND,1906)T(1),T(MPSI)
WRITE(ND,1907)U(1),U(MPSI)
WTMIX(1)=0.0
WTMIX(MPSI)=0.0
DO 1930 J=1,NS
WTMIX(1)=WTMIX(1)+ALPHA(J,1)
1930 WTMIX(MPSI)=WTMIX(MPSI)+ALPHA(J,MPSI)
DO 1919 J=1,NS
RALPHA(J,1)=ALPHA(J,1)/WTMIX(1)
RALPHA(J,MPSI)=ALPHA(J,MPSI)/WTMIX(MPSI)
1919 WRITE(ND,1917)AID(J),RALPHA(J,1),RALPHA(J,MPSI)
WRITE(ND,120)
DO 159 I=1,NR
L=IRR(I)
GO TO(131,132,133,134,135,136,137,138,139,140),L
131 J1=IRRR(I,1)
J2=IRRR(I,2)
J3=IRRR(I,3)
J4=IRRR(I,4)
WRITE(ND,121)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)
GO TO 159
132 J1=IRRR(I,1)
J2=IRRR(I,2)
J3=IRRR(I,3)
WRITE(ND,122)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
GO TO 159
133 J1=IRRR(I,1)
J2=IRRR(I,2)
J3=IRRR(I,3)
J4=IRRR(I,4)
J5=IRRR(I,5)
WRITE(ND,123)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=
11,3)
GO TO 159
134 J1=IRRR(I,1)
J2=IRRR(I,2)

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      J3=IRRR(I,3)
      WRITE(ND,124)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
135  J1=IRRR(I,1)
      J2=IRRR(I,3)
      J3=IRRR(I,4)
      WRITE(ND,125)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
136  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      WRITE(ND,126)I,AID(J1),AID(J2),AID(J3),AID(J4),(RC(I,J),J=1,3)
      GO TO 159
137  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,127)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
138  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      J4=IRRR(I,4)
      J5=IRRR(I,5)
      WRITE(ND,128)I,AID(J1),AID(J2),AID(J3),AID(J4),AID(J5),(RC(I,J),J=
11,3)
      GO TO 159
139  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,129)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
      GO TO 159
140  J1=IRRR(I,1)
      J2=IRRR(I,2)
      J3=IRRR(I,3)
      WRITE(ND,130)I,AID(J1),AID(J2),AID(J3),(RC(I,J),J=1,3)
159  CONTINUE
120  FORMAT(1H0,19X,26HREACTIONS BEING CONSIDERED,6X,19H $KR=A*EXP(B/RT)/$ 
1T**N,7X,1HA,8X,1HN,9X,1HB,7X,23H(MOLECULE-ML-SEC UNITS))
121  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,1E10.4,2X
1,F4.1,2X,F10.1)
122  FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,
1E10.4,2X,F4.1,2X,F10.1)
123  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,
1E9.3,2X,F4.1,2X,F10.1)
124  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,E9.3,2X,F4.1,2X,F10.1)
125  FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,
1E9.3,2X,F4.1,2X,F10.1)
126  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,18X,E9.3,2X,
1F4.1,2X,F10.1,3X,16HONE WAY REACTION)
127  FORMAT(I9,9X,A6,2H+ ,A6,3H+ M,5X,2H= ,A6,3H+ M,23X,
1E9.3,2X,F4.1,2X,F10.1,3X,16HONE WAY REACTION)
128  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,2H+ ,A6,2H+ ,A6,10X,
1E9.3,2X,F4.1,2X,F10.1,3X,16HONE WAY REACTION)
129  FORMAT(I9,9X,A6,2H+ ,A6,8X,2H= ,A6,26X,E9.3,2X,F4.1,2X,F10.1,3

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1X,16H ONE WAY REACTION)
130 FORMAT(I9,9X,A6,3H+ M,13X,2H= ,A6,2H+ ,A6,3H+ M,15X,E9.3,
12X,F4.1,2X,F10.1,3X,16H ONE WAY REACTION)
1901 FORMAT(1H1,37X,46H AEROCHEM RESEARCH LABORATORIES PRINCETON N.J.)
1902 FORMAT(35X,50H AXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY)
1903 FORMAT(1H0,24X,10A8)
1904 FORMAT(1H0,22X,19H PRESSURE(INITIAL) = E15.7,12H ATMOSPHERES)
1905 FORMAT(1H0,22X,20H PRESSURE(CONSTANT) = E15.7,12H ATMOSPHERES)
1906 FORMAT(23X,24H TEMPERATURE(DEG. KELVIN),3X, E15.7,4X, E15.7)
1907 FORMAT(23X,24H VELOCITY (METERS/SECOND),3X, E15.7,4X, E15.7)
1908 FORMAT(1H0,22X,14H NOZZLE RADIUS= E15.7,7H METERS)
1909 FORMAT(1H0,22X,23H LEWIS NUMBER(CONSTANT)= E15.7,5X,25H PRANDTL NUM
1BER(CONSTANT)= E15.7)
1916 FORMAT(1H0,54X,3H JET,16X,4H EDGE)
1917 FORMAT(23X,13H MOLE FRACTION,3X,A6,5X, E15.7,4X, E15.7)
1959 FORMAT(1H0,22X,40H LAMINAR VISCOSITY MODEL(SUTHERLANDS LAW))
1960 FORMAT(1H0,22X,29H CONSTANT VISCOSITY MODEL MU= E15.7)
1962 FORMAT(1H0,22X,31H TING-LIBBY VISCOSITY MODEL K= E15.7)
1961 FORMAT(1H0,22X,27H FERRI VISCOSITY MODEL K= E15.7)
1966 FORMAT(/,22X,18H X INITIAL(METERS)=,E15.7,12X,16H X FINAL(METERS)=,
*E15.7)
1967 FORMAT(1H0,22X,16H PRINT INCREMENT= E15.7,12X,18H MINIMUM STEP SIZE
1= E15.7)
9951 FORMAT(1H0,22X,69H TING-LIBBY VISCOSITY MODEL AFTER MIXING REGION I
1 INTERSECTS X AXIS K= E15.7)
X=X/AMULT
XMAX=XMAX/AMULT
PRNT=PRNT/AMULT
RJ=RJ/AMULT
DXMIN=DXMIN/AMULT
DO 7667 I=1,MPSI
7667 U(I)=U(I)/AMULT
RETURN
END
SUBROUTINE GRATE(ANSWER,Y,X,N)
DIMENSION X(30),Y(50)
COMMON/UNITS/NNDUM(15),ND
SUM = 0.0
INTER = N-1
I1 = 1
I2 = 2
DO 1 I = 1,INTER
SUM = SUM + (X(I2)-X(I1))*(Y(I2)+Y(I1))
I1 = I1 + 1
I2 = I2 + 1
1 CONTINUE
ANSWER = 0.5*SUM
RETURN
END
SUBROUTINE TICK(JJJJ)
CALL SECOND(TIME)
JJJJ=TIME
RETURN
END
SUBROUTINE SLDP(X,A,N)

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C   THIS PROGRAM FINDS THE SOLUTIONS TO A SET OF N SIMULTANEOUS LINEAR
C   EQUATIONS BY USING THE GAUSS-GORDAN REDUCTION ALGORITHM WITH THE
C   DIAGONAL PIVOT STRATEGY
      DIMENSION A(25,25),X(25)
      COMMON/UNITS/ NNDUM(14),ND,NDBG
      DO 9 K=1,N
      IF (ABS(A(K,K)) .GT. 1.E-10) GO TO 5
      WRITE(NDBG,101)
      GO TO 99
5    KP1= K+1
      DO 6 J= KP1, N
6    A(K,J)= A(K,J)/A(K,K)
      X(K)= X(K)/A(K,K)
      A(K,K)= 1.0
      DO 9 I=1,N
      IF (I.EQ.K .OR. A(I,K).EQ.0.) GO TO 9
      DO 8 J=KP1,N
8    A(I,J)= A(I,J)- A(I,K)*A(K,J)
      X(I)= X(I)- A(I,K)*X(K)
      A(I,K)=0.
9    CONTINUE
99   CONTINUE
101  FORMAT( 22H ERROR---- SMALL PIVOT )
      RETURN
      END
      SUBROUTINE TKEY(T,TTB,ITKEY,SDT,HDT,NT,J)
      DIMENSION TTB(30,24)
      COMMON/UNITS/NNDUM(15),NDBG
      NT1=NT-1
      DO 10 IT=1,NT1
      DT= TTB(IT+1,J)-TTB(IT,J)
      SDT=(T-TTB(IT,J))/DT
      HDT=(TTB( IT+1,J)-T) /DT
      IF ((SDT*HDT).GE.0.0) GO TO 11
10   CONTINUE
      WRITE(NDBG,100) T,IT
      ITKEY=0
100  FORMAT(1H , 28H  TEMPERATURE OUT OF RANGE , E14.5,I5)
      RETURN
11   ITKEY=IT
      RETURN
      END
      SUBROUTINE LIPLN(ITKEY,I,ATB,SDT,HDT,AX)
      DIMENSION ATB(25,30)
      AX= ATB(I,ITKEY)*HDT+ ATB(I,ITKEY+1)*SDT
      RETURN
      END

```

APPENDIX K  
MEFF, BLAKE, LAPP OUTPUT LISTING

155-MM HOWITZER WITH M203 CHARGE

MUZZLE VELOCITY VC = 807.7 M/SEC  
BORE LENGTH L = 5.080 METERS  
PROPELLANT MASS MP = 12.23 KG  
PROJECTILE MASS W = 46.36 KG  
GUN CALIBER CALBER = 156.5 MM  
BARREL CROSS SECTIONAL AREA A = .1924E-01 M\*\*2  
SPECIFIC HEAT RATIO OF PROPELLANT GAS GAM = 1.241  
MEAN MOLECULAR WEIGHT OF PROPELLANT GAS MBAR = 23.43  
AVERAGE BARREL GAS TEMPERATURE TA = 1860. DEG K  
COVOLUME ETA = .1041E-02 M\*\*3/KG  
CHAMBER VOLUME CVD = .1966E-01 M\*\*3

MUZZLE GAS PROPERTIES WHEN PROJECTILE IS EJECTED

PRESSURE= 694.21 ATM  
TEMPERATURE= 1828.2 K  
VELOCITY= 807.7 M/SEC

MUZZLE GAS PROPERTIES WHEN MUZZLE VELOCITY BECOMES SONIC

PRESSURE= 554.38 ATM  
TEMPERATURE= 1749.0 K  
VELOCITY= 877.7 M/SEC  
FRACTION OF EJECTED PROPELLANT= .0095

FLOW CONDITIONS AT REFLECTED SHOCK WHEN MUZZLE VELOCITY BECOMES SONIC

PRESSURE= 1.00 ATM  
TEMPERATURE= 512.8 K  
VELOCITY= 2299.8 M/SEC  
FRACTION OF GAS ENTERING REFLECTED SHOCK= .8159

FLOW CONDITIONS AT NORMAL SHOCK WHEN MUZZLE VELOCITY BECOMES SONIC

PRESSURE = 1.00 ATM  
TEMPERATURE = 1934.1 K  
VELOCITY = 306.0 M/SEC

FLOW CONDITIONS AT MIXING REGION BOUNDARY WHEN MUZZLE VELOCITY BECOMES SONIC

PRESSURE = 1.00 ATM  
TEMPERATURE = 987.9 K  
VELOCITY = 1932.8 M/SEC  
BOUNDARY RADIUS = .933 M

MACH NO IS .6E. 1

\*\* PROGRAM BLAKE, VERSION 205.11 \*\*

TIGER! TIGER! BURNING BRIGHT/ IN THE FORESTS OF THE NIGHT,  
WHAT IMMORTAL HAND OR EYE/ DARE FRAME THY FEARFUL SYMMETRY?  
---WILLIAM BLAKE (1757-1827)

25 AUG, 1983

\*\*NOTE: THE USE OF ENGLISH UNITS IS TO BE DEPRECATED. SI UNITS ARE COMING. YOU WON'T LEARN THEM IF YOU DON'T USE THEM !

\* \* USING THE BINARY LIBRARY CREATED ON 12 NOV, 1982 \* \*

M30A1

THE COMPOSITION IS

NAME	PCT WT	PCT MOLE	DEL H-CAL/M	FORMULA
NC1260	27.900	.018	-1.6916E+08	C 6000 H 7549 O 9901 N 2451
NG	22.420	17.201	-8.8600E+04	C 3 H 5 O 9 N 3
NQ	46.840	78.419	-2.2100E+04	C 1 H 4 O 2 N 4
EC	1.490	.967	-2.5100E+04	C 17 H 20 O 1 N 2
KS	1.000	1.000	-3.4266E+05	K 2 S 1 O 4
ALC	.250	.945	-6.6420E+04	C 2 H 6 O 1
C	.100	1.451	0.	C 1

THE HEAT OF FORMATION IS -384.86 CAL/GRAM = -6.7053E+04 CAL/MOLE.

THE ELEMENTS AND PERCENT BY MOLE

C	14.896
H	32.439
O	28.660
N	23.830
K	.116
S	.058

M30A1

THERE ARE 29 GASEOUS CONSTITUENTS SELECTED

NAME	BKW	L-J	EPS/K	L-J	SIGMA	A1	A2	A3	A4	A5	A6	A7	A8	A9
1. CO	390.0	91.7	3.690	3.690	5.83775	-4.0270	.06491	-.00373	-.00373	-2.14066	.71717	-.08241	-31130.5	53.1746
2. H2O	250.0	542.5	2.790	2.790	7.60069	.39388	-.10260	.00807	.00807	-4.86836	2.30899	-.37689	-62860.1	47.1008
3. CO2	600.0	195.2	3.941	3.941	9.06744	-.40694	.06138	-.00273	-.00273	-2.70529	.56199	-.04428	-102647.7	60.2574
4. N2	380.0	71.4	3.798	3.798	5.90618	-.39603	.05863	-.00307	-.00307	-2.41322	.69566	-.11540	-4589.1	51.2456
5. H2	180.0	59.7	2.827	2.827	4.48064	.19824	-.00851	-.00003	-.00003	-1.97442	1.15151	-.21216	-2116.7	36.2744
6. NO	386.0	116.7	3.492	3.492	5.77838	-.43892	.08202	-.00561	-.00561	-1.79245	.50895	-.04564	16765.3	57.0969
7. KOH	0.0	100.0	3.500	3.500	7.27052	.40176	-.10705	.00896	.00896	-1.70167	.87842	-.16291	-59999.7	68.1294
8. NH3	476.0	558.3	2.900	2.900	13.60829	-.93312	.18185	-.00958	-.00958	-9.06058	3.51672	-.50840	-22985.7	43.5074
9. HCN	359.0	344.7	3.339	3.339	9.48792	-.37343	.04424	-.00222	-.00222	-4.59416	1.73907	-.25679	24383.5	53.6459
10. CH4	528.0	148.6	3.758	3.758	20.35251	-.195871	.26284	-.01397	-.01397	-14.43248	5.11197	-.67906	-38010.8	38.5449
11. COS	0.0	100.0	3.500	3.500	9.07572	-.47894	.09730	-.00658	-.00658	-2.27231	.48548	-.04719	-41172.7	66.5255
12. C2H4	372.0	224.7	4.163	4.163	22.63477	-.164131	.20002	-.00937	-.00937	-13.78191	4.49325	-.59268	-10548.7	51.3360
13. C2H2	0.0	100.0	3.500	3.500	12.54985	-.16675	.02155	-.00023	-.00023	-5.90900	2.01409	-.26643	43014.0	54.7220
14. O2	350.0	106.7	3.467	3.467	2.20306	1.12042	-.18485	.01276	.01276	2.02364	-1.20737	-.22334	-2085.5	59.2300
15. K	0.0	100.0	3.500	3.500	6.09867	-.144727	.10388	-.03850	-.03850	-3.46738	1.37555	-.18637	16559.0	41.4178
16. S	0.0	100.0	3.500	3.500	1.83331	.19365	.01065	-.00358	-.00358	.77619	-.26477	.03824	65713.8	47.5476
17. C2N2	0.0	100.0	3.500	3.500	13.82927	-.113108	.19089	-.01258	-.01258	-5.06809	1.56648	-.19796	61813.4	70.4037
18. OH	226.0	100.0	3.500	3.500	4.22400	.47240	-.11211	.00942	.00942	-1.70189	.97134	-.16944	7437.0	49.0478
19. KO	0.0	100.0	3.500	3.500	4.49837	.11393	.00019	-.00002	-.00002	.00503	-.02588	.00186	14185.2	67.4039
20. SO	0.0	100.0	3.500	3.500	1.92172	1.33802	-.22714	.01363	.01363	2.24044	-1.13902	.18518	-219.7	63.6970
21. S2	0.0	100.0	3.500	3.500	4.48800	.03544	-.00050	.00003	.00003	.02430	-.11854	.01769	27643.9	64.5607
22. HS	0.0	100.0	3.500	3.500	6.12907	-.41325	.06726	-.00371	-.00371	-2.95581	1.32672	-.19604	30547.3	51.9361
23. CH3	525.0	100.0	3.500	3.500	13.82287	-.74765	.05695	-.00032	-.00032	-9.14376	3.65133	-.54025	23004.1	46.4265
24. H	13.4	100.0	3.500	3.500	2.49993	.00000	-.00000	.00000	.00000	.00000	-.00000	.00000	50621.8	33.4341
25. O	212.8	100.0	3.500	3.500	2.97972	-.25641	.05953	-.00389	-.00389	-.43119	.19753	-.02943	57760.7	44.3789
26. CHO	700.0	100.0	3.500	3.500	10.04357	-.109647	.20969	-.01480	-.01480	-4.57561	1.36019	-.14753	955.9	59.4686
27. CH2	525.0	100.0	3.500	3.500	11.42150	-.132276	.21610	-.01403	-.01403	-7.38097	3.01187	-.44496	83047.1	47.9048
28. CN	0.0	100.0	3.500	3.500	2.71179	.54169	.29568	-.02040	-.02040	1.50282	-1.01851	-.20537	161465.0	58.3631
29. K2	0.0	100.0	3.500	3.500	4.50198	.24737	.00004	.00000	.00000	-.00245	-.00020	-.00023	27675.0	70.3214

THE FLOOR IS AT 14

M30A1

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHO (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP	
1)	.100000E+01	6781.3218	1934.	-598.50	-762.72	2.693	.000	.357	4.187	4.181	1.240

CONSTITUENT CONCENTRATIONS - MOLES PER KG OF COMPOUND

NAME	CONCENTRATION
N2	1.17932E+01
CO	1.08207E+01
H2O	9.63504E+00
H2	6.37568E+00
CO2	3.91796E+00
KOH	5.35738E-02
COS	4.81146E-03
NO	1.00016E-04
NH3	2.97012E-05
O2	3.17973E-06
HCN	2.44635E-06
CH4	1.15941E-08
C2H4	0.
C2H2	0.
K	6.11977E-02
S	1.46775E-03
C2N2	0.
DH	2.21924E-03
KO	2.64480E-06
SO	1.46835E-02
S2	1.19222E-02
HS	1.25803E-02
CH3	0.
H	1.71882E-02
O	4.45821E-06
CHO	1.75940E-06
CH2	0.
CN	0.
K2	2.91199E-07

TOTAL GAS (MOLES/KG) 42.7226

H30A1

TRUNCATED VIRIAL EQUATION OF STATE WITH L-J 6,12 POTENTIAL IS BEING USED

P (ATM)	V (CC/GM)	T (K)	H (CAL/GM)	E (CAL/GM)	S (CAL/K/GM)	RHO (GM/CC)	CV (CAL/K)	ALPHA	BETA	ADEXP
1) .694204E+03	10.2418	1828.	-634.45	-806.63	2.111	.098	.347	3.987	3.573	1.396

CONSTITUENT CONCENTRATIONS - MOLES PER KGM OF COMPOUND

NAME	1)
N2	1.17775E+01
CO	1.06925E+01
H2O	9.54899E+00
H2	6.37242E+00
CO2	3.98099E+00
KOH	1.10894E-01
COS	5.27317E-02
NO	1.00175E-06
NH3	2.94718E-02
O2	0.
HCN	2.15448E-03
CH4	1.51000E-02
C2H4	3.37669E-06
C2H2	1.90387E-06
K	3.87803E-03
S	6.84639E-06
C2N2	3.95391E-09
OH	2.56511E-05
KO	6.79464E-08
SO	7.06865E-05
S2	9.75216E-04
H5	2.62794E-03
CH3	1.58578E-05
H	2.64819E-04
D	0.
CHO	2.79025E-05
CH2	0.
CN	2.01530E-09
K2	1.11125E-06

TOTAL GAS (MOLES/KG) 42.5903

ALPHA =	.816
H2U	2.245E-01
CO	2.515E-01
H2	1.496E-01
N2	2.765E-01
CO2	9.318E-02
H	7.920E-05
OH	1.006E-05
O	1.923E-08
O2	1.371E-08
K	3.382E-04
KOH	2.356E-03
KO2	0.
HU2	0.

AERUCHEM RESEARCH LABORATORIES PRINCETON N.J.  
AXISYMMETRIC MIXING WITH NON-EQUILIBRIUM CHEMISTRY

155-MM HOWITZER WITH H2O3 CHARGE

PRESSURE(CONSTANT) = .100000E+01 ATMOSPHERES

NOZZLE RADIUS= .933000E+00 METERS

LEWIS NUMBER(CONSTANT)= .100000E+01 PRANDTL NUMBER(CONSTANT)= .100000E+01

X INITIAL(METERS)= 0.

X FINAL(METERS)= .500000E+02

PRINT INCREMENT= .500000E+01 MINIMUM STEP SIZE= .100000E-10

DONALDSON/GRAY VISCOSITY MODEL

EDGE

JET

TEMPERATURE(DEG. KELVIN)  
VELOCITY (METERS/SECOND)

MOLE FRACTION H2O	.9878710E+03	.2940000E+03
MOLE FRACTION CO	.1932812E+04	.3000000E+01
MOLE FRACTION H2	.2249356E+00	.9996801E-51
MOLE FRACTION N2	.2519880E+00	.9996801E-51
MOLE FRACTION CO2	.1498903E+00	.9996801E-51
MOLE FRACTION H	.2770365E+00	.7897473E+00
MOLE FRACTION OH	.9336079E-01	.3198976E-03
MOLE FRACTION O	.7935367E-04	.9996801E-51
MOLE FRACTION K	.1007952E-04	.9996801E-51
MOLE FRACTION KOH	.1926731E-07	.9996801E-51
MOLE FRACTION K02	.1373660E-07	.2099328E+00
MOLE FRACTION H02	.3388562E-03	.9996801E-51
MOLE FRACTION H02	.2360571E-02	.9996801E-51
MOLE FRACTION H02	.1001940E-98	.9996801E-51
MOLE FRACTION H02	.1001940E-98	.9996801E-51

REACTIONS BEING CONSIDERED

KR=AXEXP(B/RT)/T\*\*N

(MOLECULE-ML-SEC UNITS)

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25
C0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
C0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
O	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
OH	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
O	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
OH	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
C0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
OH	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
O	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
O	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H02	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
H	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
K	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
K02	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
K	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
K02	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+
K02	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+	0	+

155-MM HOWITZER WITH M203 CHARGE

X = 0.

METERS

DELTA X METERS PRESS(ATM)  
 .933000E-01 .100000E+01

0.

HALF  
 RADIUS/R  
 .227167E+01

INNER MIXING  
 ZONE RADIUS/R  
 .112717E+01

MACH NUMBER  
 AT HALF RADIUS  
 .184557E+01

MIXING RATE  
 COEFFICIENT  
 .248000E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	0.	1
2	.1000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.220549E+01	2
3	.2000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.441098E+01	3
4	.3000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.661647E+01	4
5	.4000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.882196E+01	5
6	.5000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.110275E+02	6
7	.6000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.132329E+02	7
8	.7000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.154384E+02	8
9	.8000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.176439E+02	9
10	.9000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.198494E+02	10
11	1.0000	.193281E+04	.987871E+03	.289154E+00	.286654E+01	-.982825E+03	.738657E+01	.220549E+02	11
12	3.5433	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.305634E+02	.242604E+02	12
13	7.6940	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.305634E+02	.264659E+02	13

## 155-MM HOWITZER WITH M203 CHARGE

METERS

X= 0.

## MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	U	OH	PT
1	0.00000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	1
2	.10000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	2
3	.20000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	3
4	.30000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	4
5	.40000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	5
6	.50000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	6
7	.60000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	7
8	.70000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	8
9	.80000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	9
10	.90000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	10
11	1.00000	.22494E+00	.25199E+00	.14989E+00	.27704E+00	.93361E-01	.79354E-04	.10080E-04	11
12	3.54334	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	12
13	7.69399	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	13

155-MM HOWITZER WITH M203 CHARGE

METERS

X= 0.

MOLE FRACTIONS

PT	Y/R	O	02	K	KOH	KO2	H02	PT
1	0.00000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	1
2	.10000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	2
3	.20000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	3
4	.30000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	4
5	.40000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	5
6	.50000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	6
7	.60000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	7
8	.70000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	8
9	.80000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	9
10	.90000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	10
11	1.00000	.19267E-07	.13737E-07	.33886E-03	.23606E-02	.10019E-98	.10019E-98	11
12	3.54334	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	12
13	7.69399	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	13

## 155-MM HOWITZER WITH M203 CHARGE

.1001622E+02 METERS

X/R DELTA X METERS PRESSIATM)  
.107355E+02 .206823E-01 .10000E+01HALF INNER MIXING  
RADIUS/R ZONE RADIUS/R  
.115144E+01 .540351E+00MACH NUMBER  
AT HALF RADIUS  
.147341E+01MIXING RATE  
COEFFICIENT  
.248000E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.192714E+04	.990368E+03	.288604E+00	.285557E+01	-.978827E+03	.392487E+01	0.	1
2	.1003	.192757E+04	.990773E+03	.288530E+00	.285310E+01	-.977848E+03	.392387E+01	.220549E+01	2
3	.2007	.192075E+04	.992158E+03	.288278E+00	.284458E+01	-.974473E+03	.392044E+01	.441098E+01	3
4	.3016	.190998E+04	.995126E+03	.287741E+00	.282612E+01	-.967126E+03	.391313E+01	.651647E+01	4
5	.4032	.188914E+04	.100074E+04	.286740E+00	.279063E+01	-.952884E+03	.389953E+01	.882196E+01	5
6	.5066	.185142E+04	.101048E+04	.285064E+00	.272713E+01	-.927051E+03	.387673E+01	.110275E+02	6
7	.6128	.178696E+04	.102590E+04	.282613E+00	.262103E+01	-.883311E+03	.384340E+01	.132329E+02	7
8	.7241	.168249E+04	.104729E+04	.279783E+00	.245539E+01	-.813876E+03	.380491E+01	.154384E+02	8
9	.8437	.152236E+04	.107036E+04	.278286E+00	.221503E+01	-.711406E+03	.378456E+01	.176439E+02	9
10	.9762	.129417E+04	.107922E+04	.282661E+00	.189545E+01	-.574240E+03	.384405E+01	.198494E+02	10
11	1.1273	.100623E+04	.103625E+04	.303443E+00	.152206E+01	-.416596E+03	.412667E+01	.220549E+02	11
12	1.3025	.707100E+03	.918336E+03	.353492E+00	.114750E+01	-.271100E+03	.480732E+01	.242604E+02	12
13	1.5071	.457759E+03	.760228E+03	.438940E+00	.821422E+00	-.164616E+03	.596937E+01	.264659E+02	13
14	1.7488	.281450E+03	.608745E+03	.559271E+00	.565663E+00	-.972430E+02	.760580E+01	.286714E+02	14
15	2.0419	.166621E+03	.489951E+03	.704186E+00	.373766E+00	-.562974E+02	.957658E+01	.308769E+02	15
16	2.4167	.936390E+02	.405924E+03	.857268E+00	.230896E+00	-.318055E+02	.116584E+02	.330824E+02	16
17	2.9406	.477679E+02	.349976E+03	.999726E+00	.127043E+00	-.165480E+02	.135958E+02	.352879E+02	17
18	3.7817	.205787E+02	.316007E+03	.111078E+01	.576562E-01	-.775438E+01	.151060E+02	.374933E+02	18
19	5.3126	.790298E+01	.300098E+03	.117143E+01	.227326E-01	-.360440E+01	.159309E+02	.396988E+02	19
20	7.7739	.413328E+01	.295394E+03	.119062E+01	.119853E-01	-.236115E+01	.161919E+02	.419043E+02	20
21	10.5817	.328819E+01	.294350E+03	.119497E+01	.955199E-02	-.207973E+01	.162509E+02	.441098E+02	21
22	13.1111	.308263E+01	.294100E+03	.119601E+01	.895875E-02	-.201057E+01	.162652E+02	.463153E+02	22
23	15.4433	.302242E+01	.294027E+03	.119632E+01	.878486E-02	-.199012E+01	.162694E+02	.485208E+02	23
24	17.5407	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.162709E+02	.507263E+02	24

## 155-MM HOWITZER WITH M203 CHARGE

X = .1001622E+02 METERS

## MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.2245E+00	.25140E+00	.14951E+00	.27828E+00	.93153E-01	.70257E-07	.24896E-09	1
2	.10029	.22441E+00	.25125E+00	.14941E+00	.27859E+00	.93099E-01	.81986E-07	.29694E-08	2
3	.20070	.22397E+00	.25072E+00	.14909E+00	.27968E+00	.92913E-01	.11865E-06	.45107E-08	3
4	.30155	.22300E+00	.24959E+00	.14838E+00	.28203E+00	.92505E-01	.18415E-06	.74196E-08	4
5	.40324	.22110E+00	.24737E+00	.14701E+00	.28658E+00	.91711E-01	.28220E-06	.12122E-07	5
6	.50658	.21762E+00	.24332E+00	.14452E+00	.29486E+00	.90260E-01	.42066E-06	.19326E-07	6
7	.61284	.21159E+00	.23631E+00	.14021E+00	.30914E+00	.87750E-01	.63522E-06	.31297E-07	7
8	.72415	.20162E+00	.22472E+00	.13312E+00	.33266E+00	.83615E-01	.10764E-05	.57851E-07	8
9	.84370	.18596E+00	.20647E+00	.12191E+00	.36968E+00	.77114E-01	.24085E-05	.15113E-06	9
10	.97616	.16271E+00	.17940E+00	.10529E+00	.42461E+00	.67447E-01	.70341E-05	.61467E-06	10
11	1.12733	.13059E+00	.14356E+00	.84039E-01	.49751E+00	.54211E-01	.39724E-05	.56197E-06	11
12	1.30255	.94183E-01	.10415E+00	.61300E-01	.57779E+00	.39237E-01	.16043E-06	.43830E-07	12
13	1.50708	.62337E-01	.69215E-01	.40880E-01	.64892E+00	.26086E-01	.23163E-08	.20354E-08	13
14	1.74883	.38872E-01	.43267E-01	.25606E-01	.70173E+00	.16389E-01	.12474E-10	.49052E-10	14
15	2.04187	.23122E-01	.25775E-01	.15273E-01	.73732E+00	.98784E-02	.36111E-13	.64481E-12	15
16	2.41673	.12909E-01	.14405E-01	.85428E-02	.76045E+00	.56566E-02	.95285E-16	.66033E-14	16
17	2.94058	.64075E-02	.71549E-02	.42455E-02	.77520E+00	.29688E-02	.36170E-18	.86119E-16	17
18	3.78168	.25232E-02	.28190E-02	.16734E-02	.78401E+00	.13630E-02	.23631E-20	.20075E-17	18
19	5.31257	.70463E-03	.78752E-03	.46763E-03	.78815E+00	.61120E-03	.26463E-22	.94573E-19	19
20	7.77393	.16290E-03	.18213E-03	.10818E-03	.78938E+00	.38725E-03	.24551E-23	.39789E-17	20
21	10.58171	.41423E-04	.46322E-04	.27519E-04	.78965E+00	.33702E-03	.13339E-23	.86313E-19	21
22	13.11106	.11876E-04	.13283E-04	.78920E-05	.78972E+00	.32481E-03	.31483E-24	.70957E-19	22
23	15.44331	.32214E-05	.36033E-05	.21411E-05	.78974E+00	.32123E-03	.36408E-25	.30280E-19	23
24	17.54072	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	24

X= .1001622E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

## MOLE FRACTIONS

P.T	Y/R	D	O2	K	KOH	KO2	H2O2	P.T
1	0.00000	.34911E-10	.43172E-03	.37470E-03	.22662E-02	.52256E-04	.10977E-06	1
2	.10029	.51761E-10	.54617E-03	.36513E-03	.22648E-02	.61653E-04	.15389E-06	2
3	.20070	.13081E-09	.94454E-03	.33567E-03	.22598E-02	.90595E-04	.32192E-06	3
4	.30155	.39885E-09	.18270E-02	.28555E-03	.22485E-02	.13992E-03	.73271E-06	4
5	.40324	.12256E-08	.35752E-02	.21945E-03	.22255E-02	.20544E-03	.15684E-05	5
6	.50658	.36231E-08	.68134E-02	.15114E-03	.21810E-02	.27519E-03	.30343E-05	6
7	.61284	.10689E-07	.12472E-01	.98595E-04	.20984E-02	.33588E-03	.54796E-05	7
8	.72415	.35106E-07	.21850E-01	.72611E-04	.19506E-02	.38663E-03	.10193E-04	8
9	.84370	.15111E-06	.36621E-01	.73143E-04	.17003E-02	.44276E-03	.21999E-04	9
10	.97616	.81789E-06	.58556E-01	.90222E-04	.13353E-02	.50329E-03	.52117E-04	10
11	1.12733	.77167E-06	.88474E-01	.30925E-04	.10678E-02	.44604E-03	.73217E-04	11
12	1.30255	.42813E-07	.12218E+00	.11203E-05	.84148E-03	.27670E-03	.45865E-04	12
13	1.50708	.83956E-09	.15179E+00	.98037E-08	.58292E-03	.16019E-03	.23757E-04	13
14	1.74883	.18056E-10	.17366E+00	.23216E-10	.37282E-03	.91413E-04	.11746E-04	14
15	2.04187	.58936E-12	.18835E+00	.20122E-13	.22518E-03	.51263E-04	.57105E-05	15
16	2.41673	.22873E-13	.19788E+00	.15164E-16	.12696E-03	.27494E-04	.26767E-05	16
17	2.94058	.92065E-15	.20395E+00	.24435E-19	.63437E-04	.13266E-04	.11388E-05	17
18	3.78168	.36116E-16	.20758E+00	.67072E-22	.25099E-04	.51169E-05	.39015E-06	18
19	5.31257	.17315E-17	.20927E+00	.22124E-24	.70339E-05	.14066E-05	.95690E-07	19
20	7.77393	.15576E-17	.20978E+00	.48725E-26	.16306E-05	.32117E-06	.19513E-07	20
21	10.58171	.45314E-17	.20989E+00	.67919E-27	.41549E-06	.80902E-07	.44301E-08	21
22	13.11106	.41305E-17	.20992E+00	.49374E-28	.11928E-06	.23049E-07	.11633E-08	22
23	15.44331	.18697E-17	.20993E+00	.27455E-29	.32381E-07	.62301E-08	.29899E-09	23
24	17.54072	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	24

155-MM HOWITZER WITH M203 CHARGE

X= .1528463E+02 METERS

X/R DELTA X METERS PRESS(ATM)  
 .163822E+02 .559850E-01 .10000E+01

HALF  
 RADIUS/R  
 .136568E+01

INNER MIXING  
 ZONE RADIUS/R  
 .423064E+00

MACH NUMBER  
 AT HALF RADIUS  
 .108226E+01

MIXING RATE  
 COEFFICIENT  
 .253723E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.184212E+04	.102239E+04	.282216E+00	.270083E+01	-.920967E+03	.578919E+01	0.	1
2	.2100	.182014E+04	.103968E+04	.278395E+00	.265172E+01	-.906808E+03	.571081E+01	.441098E+01	2
3	.4279	.174858E+04	.112531E+04	.260475E+00	.247059E+01	-.863678E+03	.534322E+01	.882196E+01	3
4	.6805	.160169E+04	.139032E+04	.218487E+00	.208955E+01	-.790092E+03	.448191E+01	.132329E+02	4
5	.9949	.133226E+04	.165183E+04	.194340E+00	.164917E+01	-.668194E+03	.398656E+01	.175439E+02	5
6	1.4211	.861339E+03	.205680E+04	.170414E+00	.100413E+01	-.415905E+03	.349576E+01	.220549E+02	6
7	1.9766	.477823E+03	.121281E+04	.285225E+00	.704572E+00	-.216745E+03	.585092E+01	.254659E+02	7
8	2.4337	.267291E+03	.677657E+03	.506121E+00	.512861E+00	-.955539E+02	.103823E+02	.308762E+02	8
9	2.9690	.143056E+03	.485161E+03	.713953E+00	.323042E+00	-.479955E+02	.146456E+02	.352879E+02	9
10	3.6754	.683061E+02	.381366E+03	.915418E+00	.173935E+00	-.228944E+02	.187783E+02	.395988E+02	10
11	4.8835	.260869E+02	.324552E+03	.108086E+01	.721078E-01	-.929929E+01	.221721E+02	.441098E+02	11
12	7.3260	.831827E+01	.300970E+03	.116799E+01	.238923E-01	-.367103E+01	.239593E+02	.485208E+02	12
13	11.5966	.396635E+01	.295254E+03	.119121E+01	.115041E-01	-.229116E+01	.244358E+02	.529318E+02	13
14	16.5122	.317675E+01	.294253E+03	.119537E+01	.928795E-02	-.204571E+01	.245211E+02	.573428E+02	14
15	20.7953	.304371E+01	.294056E+03	.119620E+01	.884631E-02	-.199657E+01	.245380E+02	.617537E+02	15
16	24.7941	.300588E+01	.294008E+03	.119640E+01	.873709E-02	-.198635E+01	.245422E+02	.661647E+02	16
17	28.3697	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.245428E+02	.705757E+02	17

155-MM HOWITZER WITH M203 CHARGE

X= .1528463E+02 METERS

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	OH	PT
1	0.00000	.21805E+00	.24200E+00	.14294E+00	.29713E+00	.90463E-01	.71503E-06	.32498E-07	1
2	.21004	.21764E+00	.23898E+00	.14029E+00	.30227E+00	.90538E-01	.13845E-05	.53269E-07	2
3	.42789	.21950E+00	.22674E+00	.12924E+00	.31997E+00	.93837E-01	.32376E-04	.80314E-06	3
4	.68049	.22673E+00	.18722E+00	.10394E+00	.36108E+00	.11707E+00	.11205E-02	.43026E-04	4
5	.99490	.22694E+00	.12832E+00	.63712E-01	.43874E+00	.13910E+00	.46524E-03	.73167E-04	5
6	1.42109	.19958E+00	.14888E-01	.30828E-02	.58813E+00	.17377E+00	.50816E-03	.35869E-02	6
7	1.97658	.11017E+00	.38208E-01	.11991E-02	.66812E+00	.64931E-01	.33668E-03	.44997E-03	7
8	2.43368	.42771E-01	.35496E-01	.18879E-01	.71014E+00	.21562E-01	.15228E-06	.15228E-06	8
9	2.96901	.21043E-01	.20961E-01	.11954E-01	.74563E+00	.97240E-02	.13237E-10	.28125E-09	9
10	3.67539	.95688E-02	.10204E-01	.59389E-02	.76875E+00	.43865E-02	.37528E-14	.47145E-12	10
11	4.88349	.33516E-02	.36719E-02	.21571E-02	.78225E+00	.17171E-02	.18447E-17	.11168E-14	11
12	7.32596	.76910E-03	.85153E-03	.50250E-03	.78801E+00	.63853E-03	.14115E-20	.46683E-17	12
13	11.59658	.13945E-03	.15506E-03	.91720E-04	.78943E+00	.37757E-03	.39004E-23	.76359E-19	13
14	16.51219	.28360E-04	.31593E-04	.18711E-04	.78968E+00	.33162E-03	.26048E-24	.24576E-19	14
15	20.79530	.62969E-05	.70210E-05	.41610E-05	.78973E+00	.32250E-03	.26372E-25	.11249E-19	15
16	24.79405	.84699E-06	.94462E-06	.55994E-06	.78975E+00	.32025E-03	.57471E-27	.18534E-20	16
17	28.36967	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	17

155-MM HOWITZER WITH M203 CHARGE

X= .1528463E+02 METERS

MOLE FRACTIONS

PT	Y/R	U	OZ	K	KOH	KO2	H32	PT
1	0.00000	.65801E-08	.68086E-02	.23080E-03	.19991E-02	.36870E-03	.62387E-05	1
2	.21004	.16256E-07	.76922E-02	.42879E-03	.17291E-02	.41767E-03	.10038E-04	2
3	.42789	.50663E-06	.81553E-02	.15391E-02	.55795E-03	.40858E-03	.23864E-04	3
4	.68049	.18781E-05	.41519E-03	.22981E-02	.76232E-04	.37400E-05	.41223E-06	4
5	.99490	.18626E-05	.54475E-03	.17425E-02	.34627E-03	.82884E-06	.23408E-06	5
6	1.42109	.45270E-03	.14518E-01	.42459E-03	.10482E-02	.44536E-06	.21954E-05	6
7	1.97658	.57037E-03	.11516E+00	.26740E-03	.52929E-03	.76444E-05	.54701E-04	7
8	2.43368	.57584E-06	.17064E+00	.22065E-06	.30555E-03	.13812E-03	.68413E-04	8
9	2.96901	.19624E-08	.19042E+00	.52212E-10	.17181E-03	.65752E-04	.22405E-04	9
10	3.67539	.43098E-11	.20104E+00	.17842E-14	.83944E-04	.27702E-04	.68821E-05	10
11	4.88349	.13658E-13	.20681E+00	.95071E-19	.30714E-04	.89459E-05	.16469E-05	11
12	7.32596	.74520E-16	.20922E+00	.15798E-22	.72429E-05	.19121E-05	.27711E-06	12
13	11.59658	.13967E-17	.20980E+00	.79702E-26	.13371E-05	.32729E-06	.39848E-07	13
14	16.51219	.55793E-18	.20991E+00	.11599E-27	.27506E-06	.63848E-07	.68988E-08	14
15	20.79530	.29133E-18	.20993E+00	.52551E-29	.61478E-07	.13817E-07	.13852E-08	15
16	24.79405	.49719E-19	.20993E+00	.40762E-30	.82863E-08	.18434E-08	.18031E-09	16
17	28.36967	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	17

X= .4196607E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

X/R DELTA X METERS PRESS(ATM)  
 .449797E+02 .110148E+00 .100000E+01

HALF INNER MIXING  
 RADIUS/R ZONE RADIUS/R  
 .223268E+01 0.

MACH NUMBER  
 AT HALF RADIUS  
 .663500E+00

MIXING RATE  
 COEFFICIENT  
 .340269E-01

PT	Y/R	VELOCITY METERS/SEC	TEMPERATURE K	DENSITY GM/CC	MACH NO.	ENTHALPY CAL/GM	VISCOSITY KG/M/SEC	PSI	PT
1	0.0000	.102834E+04	.208426E+04	.164578E+00	.117919E+01	-.486691E+03	.597887E+01	0.	1
2	.7658	.945981E+03	.216348E+04	.161016E+00	.107504E+01	-.440738E+03	.584949E+01	.882 196E+01	2
3	1.5946	.695635E+03	.201723E+04	.175091E+00	.819497E+00	-.286563E+03	.636079E+01	.176 439E+02	3
4	2.5843	.416490E+03	.146771E+04	.240453E+00	.567491E+00	-.161503E+03	.873533E+01	.264 659E+02	4
5	3.6764	.239610E+03	.100857E+04	.349043E+00	.387642E+00	-.906074E+02	.126802E+02	.352 879E+02	5
6	4.9171	.141692E+03	.720142E+03	.488249E+00	.267612E+00	-.529413E+02	.177374E+02	.441 098E+02	6
7	6.3288	.864524E+02	.548144E+03	.641202E+00	.185538E+00	-.323228E+02	.232940E+02	.529 318E+02	7
8	8.0105	.533971E+02	.443992E+03	.791602E+00	.126738E+00	-.201056E+02	.287578E+02	.617 537E+02	8
9	10.0896	.325687E+02	.379379E+03	.926556E+00	.834340E-01	-.126108E+02	.336605E+02	.705 757E+02	9
10	12.8172	.191469E+02	.339070E+03	.103692E+01	.518511E-01	-.772865E+01	.376697E+02	.793 977E+02	10
11	16.5906	.107751E+02	.314941E+03	.111657E+01	.302672E-01	-.472768E+01	.405636E+02	.882 196E+02	11
12	21.9252	.617826E+01	.302252E+03	.116362E+01	.177128E-01	-.309734E+01	.422726E+02	.970 416E+02	12
13	28.8986	.415070E+01	.296882E+03	.118476E+01	.120064E-01	-.238384E+01	.430405E+02	.105 864E+03	13
14	36.6702	.340480E+01	.294981E+03	.119243E+01	.988031E-02	-.212297E+01	.433192E+02	.114 686E+03	14
15	44.3431	.314328E+01	.294338E+03	.119505E+01	.913129E-02	-.203198E+01	.434144E+02	.123 507E+03	15
16	51.6685	.304775E+01	.294110E+03	.119598E+01	.885723E-02	-.199892E+01	.434482E+02	.132 329E+03	16
17	58.6048	.301166E+01	.294027E+03	.119632E+01	.875360E-02	-.198647E+01	.434607E+02	.141 151E+03	17
18	65.2400	.300000E+01	.294000E+03	.119643E+01	.872011E-02	-.198245E+01	.434647E+02	.149 973E+03	18

X= .4196607E+02 METERS 155-MM HOWITZER WITH M203 CHARGE

MOLE FRACTIONS

PT	Y/R	H2O	CO	H2	N2	CO2	H	CH	PT
1	0.00000	.22492E+00	.50940E-01	.13927E-01	.53772E+00	.16955E+00	.36602E-03	.66795E-03	1
2	.76580	.21640E+00	.26531E-01	.60640E-02	.56481E+00	.17965E+00	.46492E-03	.21430E-02	2
3	1.59460	.16485E+00	.16982E-02	.35128E-03	.63132E+00	.15177E+00	.46673E-04	.22319E-02	3
4	2.58433	.99050E-01	.25953E-03	.16392E-04	.69592E+00	.91414E-01	.12021E-05	.25361E-03	4
5	3.67641	.55988E-01	.18069E-02	.62228E-03	.73534E+00	.50657E-01	.33828E-07	.67960E-06	5
6	4.91710	.32200E-01	.22370E-02	.94178E-03	.75720E+00	.28611E-01	.29983E-10	.13370E-08	6
7	6.32882	.18993E-01	.20795E-02	.94100E-03	.76973E+00	.16602E-01	.30201E-13	.47274E-11	7
8	8.01054	.11240E-01	.16922E-02	.79803E-03	.77740E+00	.97160E-02	.58930E-16	.26315E-13	8
9	10.08959	.64622E-02	.12404E-02	.60190E-03	.78235E+00	.55860E-02	.27323E-18	.29197E-15	9
10	12.81720	.34579E-02	.80777E-03	.40062E-03	.78563E+00	.30659E-02	.31693E-20	.75441E-17	10
11	16.59061	.16313E-02	.44969E-03	.22705E-03	.78773E+00	.15818E-02	.81451E-22	.44050E-18	11
12	21.92523	.65336E-03	.20764E-03	.10642E-03	.78891E+00	.81198E-03	.40983E-23	.54566E-19	12
13	28.89857	.23195E-03	.83184E-04	.43163E-04	.78944E+00	.49007E-03	.34326E-24	.12054E-19	13
14	36.67017	.80165E-04	.31720E-04	.16620E-04	.78964E+00	.37731E-03	.39067E-25	.36687E-20	14
15	44.34315	.27963E-04	.11921E-04	.62911E-05	.78971E+00	.33952E-03	.50332E-26	.12660E-20	15
16	51.66853	.92256E-05	.41328E-05	.21912E-05	.78973E+00	.32628E-03	.58270E-27	.42383E-21	16
17	58.60479	.22416E-05	.10273E-05	.54583E-06	.78974E+00	.32144E-03	.35450E-28	.10408E-21	17
18	65.23998	.99968E-51	.99968E-51	.99968E-51	.78975E+00	.31990E-03	.99968E-51	.99968E-51	18

155-MM HOWITZER WITH M203 CHARGE

X= .4196607E+02 METERS

MOLE FRACTIONS

PT	Y/R	O	D2	K	KOH	KO2	H2O	PT
1	0.00000	.13158E-04	.17573E-03	.58197E-03	.11404E-02	.14053E-07	.42324E-07	1
2	.76580	.11998E-03	.22158E-02	.48220E-03	.11280E-02	.92910E-07	.42180E-06	2
3	1.59460	.22183E-03	.46308E-01	.98599E-04	.10987E-02	.72977E-06	.22273E-05	3
4	2.58433	.24432E-04	.11234E+00	.39262E-05	.70995E-03	.72970E-06	.16248E-05	4
5	3.67641	.26033E-06	.15516E+00	.59177E-07	.40074E-03	.70912E-05	.23373E-04	5
6	4.91710	.70042E-09	.17855E+00	.38192E-10	.23091E-03	.78889E-05	.19004E-04	6
7	6.32882	.15767E-11	.19149E+00	.98526E-14	.13655E-03	.70852E-05	.13870E-04	7
8	8.01054	.30454E-14	.19906E+00	.35362E-17	.81067E-04	.56718E-05	.94679E-05	8
9	10.08959	.51244E-17	.20370E+00	.65413E-20	.46783E-04	.41153E-05	.60370E-05	9
10	12.81720	.77894E-20	.20661E+00	.45568E-22	.25142E-04	.26583E-05	.34991E-05	10
11	16.59061	.14976E-22	.20837E+00	.68428E-24	.11921E-04	.14684E-05	.17611E-05	11
12	21.92523	.21295E-24	.20931E+00	.16960E-25	.48013E-05	.67257E-06	.74400E-06	12
13	28.89857	.15845E-25	.20971E+00	.65743E-27	.17148E-05	.26721E-06	.27584E-06	13
14	36.67017	.17986E-26	.20986E+00	.50917E-28	.59615E-06	.10110E-06	.98600E-07	14
15	44.34315	.24265E-27	.20991E+00	.99586E-29	.20901E-06	.37750E-07	.35244E-07	15
16	51.66853	.37509E-28	.20992E+00	.29440E-29	.69217E-07	.13028E-07	.11812E-07	16
17	58.60479	.13487E-28	.20993E+00	.70710E-30	.16848E-07	.32316E-08	.28906E-08	17
18	65.23998	.99968E-51	.20993E+00	.99968E-51	.99968E-51	.99968E-51	.99968E-51	18

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